FY17 Status Report on the Micromechanical Finite Element Modeling of Creep Fracture of Grade 91 Steel

Nuclear Engineering Division

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ABSTRACT

Advanced reactors designed to operate at higher temperatures than current light water reactors require structural materials with high creep strength and creep-fatigue resistance to achieve long design lives. Grade 91 is a ferritic/martensitic steel designed for long creep life at elevated temperatures. It has been selected as a candidate material for sodium fast reactor intermediate heat exchangers and other advanced reactor structural components. This report focuses on the creep deformation and rupture life of Grade 91 steel.

The time required to complete an experiment limits the availability of long-life creep data for Grade 91 and other structural materials. Design methods often extrapolate the available shorter-term experimental data to longer design lives. However, extrapolation methods tacitly assume the underlying material mechanisms causing creep for long-life/low-stress conditions are the same as the mechanisms controlling creep in the short-life/high-stress experiments. A change in mechanism for long-term creep could cause design methods based on extrapolation to be non-conservative.

The goal for physically-based microstructural models is to accurately predict material response in experimentally-inaccessible regions of design space. An accurate physically-based model for creep represents all the material mechanisms that contribute to creep deformation and damage and predicts the relative influence of each mechanism, which changes with loading conditions. Ideally, the individual mechanism models adhere to the material physics and not an empirical calibration to experimental data and so the model remains predictive for a wider range of loading conditions.

This report describes such a physically-based microstructural model for Grade 91 at 600° C. The model explicitly represents competing dislocation and diffusional mechanisms in both the grain bulk and grain boundaries. The model accurately recovers the available experimental creep curves at higher stresses and the limited experimental data at lower stresses, predominately primary creep rates. The current model considers only one temperature. However, because the model parameters are, for the most part, directly related to the physics of fundamental material processes, the temperature dependence of the properties are known. Therefore, temperature dependence can be included in the model with limited additional effort.

The model predicts a mechanism shift for 600° C at approximately 100 MPa from a dislocation-dominated regime at higher stress to a diffusion-dominated regime at lower stress. This mechanism shift impacts the creep life, notch-sensitivity, and, likely, creep ductility of Grade 91. In particular, the model predicts existing extrapolation methods for creep life may be non-conservative when attempting to extrapolate data for higher stress creep tests to low stress, long-life conditions. Furthermore, the model predicts a transition from notch-strengthening behavior at high stress to notch-weakening behavior at lower stresses. Both behaviors may affect the conservatism of existing design methods.

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1 Introduction

1.1 Background

Grade 91 is a ferritic/martensitic steel developed at Oak Ridge National Laboratory and Combustion Engineering for improved creep life in high temperature Liquid Metal Reactors [1] [2]. To improve the economics of plant construction many current advanced reactor concept designs consider 60-year design lives [3], requiring Grade 91 and other high temperature, high creep strength advanced alloys to maintain adequate design margins against creep deformation, creep rupture, and creep-fatigue damage.

The time required to complete an experiment necessarily limits the available creep data available for a particular material. Sixty-year experiments are not practical and so designers must extrapolate long-term creep properties from shorter term, higher stress experiments. Such extrapolation procedures necessarily assume that the deformation mechanisms controlling creep deformation and rupture processes in the extrapolated regime are the same as the controlling mechanisms in the shorter-term experiments. Potentially, under long-term creep conditions different material mechanisms govern the processes of material deformation and failure. If so, this could render extrapolation methods based on short-term data non-conservative.

Of particular concern for Grade 91 are long-term creep ductility and notch sensitivity. At higher loads Grade 91 typically undergoes ductile creep failure. However, some experiments at lower stress show limited ductility, with reduction in area on the order of a few percent. Limited creep ductility is a direct concern for design and this data could indicate a change in mechanism that could affect the conservatism of typical extrapolation procedures. Recently, the Electric Power Research Institute (EPRI) attributed the low creep ductility to chemistry effects and recommended a new grade for Grade 91 steel with restricted chemistry to resolve the low creep ductility issues. Similarly, at higher loading stresses Grade 91 is notch strengthening [4], i.e. the presence of a notch increases the experimental rupture life. However, there is experimental evidence that for severe notches Grade 91 becomes notch weakening, which could suggest a similar transition to notch-weakening behavior at lower loading stresses [5].

Experiments cannot directly test long sixty-year design lives. An alternative approach for examining long-term creep behavior is a physically-based microstructural model. Such a model captures the relevant microscale deformation mechanisms causing creep and creep rupture and extends this microscale model to simulate macroscale properties. In Grade 91 the relevant creep deformation mechanisms operate on the mesoscale – the scale of crystalline grains and grain boundaries. Crystal plasticity (CP) models deformation on this length scale and this report describes a crystal plasticity model for creep deformation in Grade 91, aimed at capturing all relevant creep deformation mechanisms in the material and accurately representing long term creep. The final complete model for Grade 91 couples this CP representation of deformation in the grain bulk with a physically based model for creep damage on the material grain boundaries (GBs). The damage model represents both creep/dislocation and diffusional void growth mechanisms and includes a framework for establishing stress and/or strain-based void nucleation criteria.

Grade 91 has a complex microstructure and so the composite model must focus on a few relevant deformation mechanisms and a particular level of the hierarchical Grade 91 structure. The

goal of the model is to capture the most important deformation modes in order to examine how the balance of deformation mechanisms changes with loading stress and triaxiality. The model retains a strong link to the physics underlying the deformation mechanisms so that its predictions can be extrapolated to long-term behavior. The model must, at some point, be calibrated to the available short-term test data, but a physically based modeling approach can account for mechanism changes in the long-life, low-stress regime where conventional extrapolation procedures might fail to produce conservative predictions of creep properties.

The model represents the important mechanisms of creep and creep rupture in both the grain bulk and the grain boundaries. This report describes validating the model against the available experimental short-life creep data as well as some data at low stress conditions, in particular primary creep rates. The validated model is then used to predict creep behavior for long-life conditions.

1.2 Creep mechanisms in Grade 91

Grade 91 has a hierarchical microstructure. At the highest level are collections of martensitic blocks arranged inside a prior austenite grain (PAG) [6] [7]. Each block represents a different austenite to martensite lattice transformation, starting from the same PAG, and so the orientations of the laths inside each PAG are correlated. Blocks are typically aligned in parallel groups called packets and several packets form inside each PAG. Tempering separates each block into a collection of parallel laths [8]. These laths can be viewed as subgrains as the misorientation between each lath in a block is much less than the misorientation between different blocks. This hierarchical structure scales from PAGs on the order of 30 μm down to the laths with a width of about 0.2 μm . Figure 1-1 shows a sketch of this structure. Note that only the PAGs and packets are approximately equiaxed, the block and lath structures are laminar.

Initial dislocation density in Grade 91 is high – around 10^{13} m^{-2} [7]. The lath subgrain boundaries themselves can be viewed as a dense dislocation network. A variety of carbides and nitrides pepper the microstructure. M_{23}C_6 , where M is an alloying species, precipitates cluster on grain boundaries [6] [7]. These precipitates, which have diameters on the order of 100 nm [9], play a key role in the increased creep strength of Grade 91. Finer precipitates, on the order of 20 nm, are more uniformly distributed throughout the microstructure, often of the form MC or MN.

This high initial defect density means that the structure tends to relax and coarsen under deformation, particularly at high temperature. The dislocation structure recovers, leading to substantial coarsening of the laths and a reduction in the overall dislocation density [10]. This leads to the macroscale softening commonly observed in uniaxial and cyclic tests on Grade 91.

Creep deformation in the Grade 91 takes place via two categories of mechanisms: dislocation motion and point defect diffusion, the exact form of which is debated in the literature. Because of the high initial dislocation density the kinetics of dislocation climb and other recovery mechanisms largely govern dislocation motion [9]. Both climb and the diffusional mechanism are thermally activated, so the interplay of the two mechanisms will be controlled by both temperature and the stress on the material. These deformation mechanisms, combined with thermal aging, cause and interact with the microstructural changes described above.

This work approximates the net effect of several diffusional mechanisms with a simple linear viscous deformation rate active in the grain bulk. In actuality, vacancies use grain boundaries and

other defect structures as diffusional highways, as the reduced lattice coherence in these regions increases their effective diffusivity. However, the model developed here only explicitly represents the highest level of the hierarchical microstructure: the prior austenite grains. Each PAG contains many packet, block, and lath subboundaries. The model developed here for grain bulk deformation must average the effect of these subboundaries into a homogeneous model for grain bulk deformation in a single, oriented PAG. For diffusional mechanisms, a reasonable approach is to assume the defect network is uniformly geometrically distributed, resulting in effective isotropic diffusion on the scale of a PAG.

While these interacting mechanisms are active in the PAG bulk the state of the grain boundaries also evolves as deformation progresses. There is an extensive literature on creep damage, which will not be summarized in detail here. Suffice to say both diffusional and dislocation-based mechanisms can, with time, grow existing voids on the grain boundaries and nucleate new voids, leading to void coalesce and creep damage that eventually causes rupture [10] [11]. These grain boundary processes are intrinsically linked to the processes occurring in the grain bulk, and so a complete grain boundary model must include information about the state of adjacent grains.

To summarize, the key creep mechanisms in Grade 91 are bulk grain motion mediated by dislocations, bulk motion mediated by variety of diffusional processes (approximated here as isotropic diffusion in the grain bulk), and void nucleation, growth, and coalesce on grain boundaries, which themselves can be mediated by either dislocation or diffusional processes. These are the key features that the crystal plasticity model in this reports aims to capture, focusing on the highest scale of the microstructure, the PAGs.

1.3 Report outline

Including this introduction and a concluding section this report divides the work into eight chapters. The general approach is to briefly summarize previous project results on a particular topic and then focus in more detail on the accomplishments of the current reporting period. The report overall describes a complete microstructural model for Grade 91 at 600° C, one that encompasses all relevant microstructural creep mechanisms, matches available experimental data, and can provide confident predictions for the creep response of Grade 91 for low stress, long-life, experimentally inaccessible conditions.

Chapter 2 summarizes work on the grain boundary model. This model, embedded on grain boundaries using cohesive-interface elements, represents the dislocation- and diffusion mediated nucleation, growth, and coalescence of voids leading to creep damage in the material. The current year's work focuses on numerical improvements to the model to increase the stability of the overall simulation framework and to extend the simulations farther into the tertiary creep regime.

The next chapter describes the final model for grain bulk deformation. The composite model includes terms representing two mechanisms: creep deformation via dislocation motion, heavily mediated by recovery processes, and a bulk, isotropic diffusional mechanism designed to homogenize the effect of vacancy diffusion along the dense, interlocking network of dislocations and subgrain boundaries inside a single PAG. Additionally, this chapter describes an alternate, dislocation density-based crystal plasticity formulation developed in the current reporting period and compares and contrasts it to the final, more empirical approach adopted for the final model.

Chapter 4 highlights a particular numerical issue encountered in polycrystal simulations including sliding grain boundaries: singular and oscillating GB traction fields resulting from the near-Hertzian contact conditions at triple points where one grain slides into another. This can be viewed as the problem of tuning an appropriate penalty stiffness to describe this contact. The report describes the process used to tune this penalty stiffness and reports the optimal value used in the complete model.

Then the report describes the effect of the representative volume element (RVE) geometry and boundary conditions. Previous project work considers block RVEs, essentially taking a representative region of microstructure and artificially slicing out a cube to use as the simulation domain. With periodic boundary conditions this method results in artificial grain boundaries on the RVE faces that are not necessarily representative of the actual microstructure. Alternatively, an RVE can be a true periodic structure of grains generated through periodic Voronoi tessellation. Such structures do not have artificial boundaries on the periodic cell edges but require sophisticated algorithms to insert cohesive elements representing the GBs and more complicated, but more general, periodic boundary conditions. Ultimately, the work described here shows both types of cells produce nearly identical results for higher applied loads. There are minor differences in the primary creep regime and at lower stresses, but these differences are not sufficient to justify the increased complexity of the true periodic cells.

Chapter 6 then describes the complete microstructural model for creep deformation in Grade 91. The section describes the process of calibrating and selecting material properties from available experimental data and validates the model against available creep curves. A key result emerges: at 600° C the model predicts a shift in mechanism from dislocation-dominated creep above 100 MPa to diffusion-dominated creep below 100 MPa. This mechanism shift also appears in experimental measurements of primary creep rate. The mechanism shift affects the microstructural details of creep, the macroscale creep curves, and times to the onset of tertiary creep. Plots of minimum creep rate versus stress illustrate potential problems extrapolating higher stress experimental data into the low stress, long life regime. Furthermore, because the model is physically based, parameters describing the final void density and void size can be compared to experiments. Both the model and experiments show a transition from larger numbers of smaller voids in the dislocation-dominated regime to fewer, larger voids in the diffusion regime, thus validating the model predictions.

The penultimate chapter applies the validated, microstructural model to notch effects. Available high stress creep tests show notch-strengthening behavior in Grade 91. The model matches the results of these experiments, showing notch strengthening behavior for high axial loads. However, at lower loads the model predicts notch strengthening for moderate notches with a transition to notch weakening for more severe triaxial stress states. Finally, at low loads in the diffusion regime the model predicts Grade 91 will be notch weakening. This is a key result, as it affects the design of Grade 91 structures with long design lives – most existing design methodologies assume notch strengthening behavior. A simple microstructural model elucidates the simulation trends, both for increasing/decreasing axial stress and notch severity, in terms of a mechanism shift between dislocation and diffusion mediated creep. These results illustrate the power of a physically-based model – once validated it can accurately simulate loading conditions difficult to reach experimentally and reveal material behavior that may have a critical impact on the design and construction of advanced reactors.

Finally, the report concludes with a chapter summarizing the important results of the project and suggesting areas for future research.

1.4 Chapter figures

Figure 1-1. Schematic describing the microstructure of Grade 91.

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2 Grain Boundary Modeling

2.1 Overview of constitutive model for grain boundaries

The constitutive modeling of grain boundary deformation in this work focuses on the creep behavior of martensitic steels of the Grade 91 class and similar alloys at high temperatures (550-650 °C). Previous work, e.g., [12] provide detailed accounts of the experimental testing and results that elucidate the deformation mechanisms that govern long term creep under the conditions in the materials of interest. The major mechanisms are summarized below and the modeling procedures follow.

The prior austenite grain boundaries (PAGBs) in Grade 91 type alloys contribute to the overall deformation of a specimen through tangential sliding and normal-direction opening mechanisms. The grain boundary sliding adds to the creep straining over the entire life and is especially significant at lower applied stresses. The opening deformation of PAGBs is ascribed to cavity formation, growth, and coalescence. During primary and secondary creep phases, the stress concentrations at particles and triple points nucleate small cavities. Under continued loading, these cavities on the PAGBs will grow and eventually coalesce to form microcracks which drive the tertiary creep phase.

The modeling approach employs an interface cohesive model with distinct sliding and cavitation responses to explicitly meshed PAGBs. This model defines the traction-separation relationships of initially zero-thickness 2D interface elements on the boundaries of the 3D prior austenite grains. The basis of the model follows the work of Needleman and Rice [86], Sham and Needleman [87], Ashby and co-workers [13], Tvergaard and van der Giessen [11], and more recently by Sham and co-workers, e.g., [12]. The current project has integrated these models into the three dimensional finite element program WARP3D [14]. Previous reports, e.g., [12] detail this implementation and extensive prior studies that elucidate many features of the model. The current report focuses on summarizing the numerical model (Section 2.1), presenting the recent implementation improvements (Section 2.2), and mapping the effects of the individual input parameters along with recommended values (Section 2.3).

2.1.1 Cavity nucleation and growth

The normal separation of the interface-cohesive model includes contributions from (1) the growth of existing cavities on the grain boundary, (2) the nucleation of new grain boundary cavities, and (3) creep deformation in neighboring grains. Figure 2-1 along with Table 2-1 and Table 2-2 introduce the variables and parameters in the normal traction-separation relationship. The separation rate, $\dot{\delta}$, depends on the volumetric growth rate and spacing of cavities on the grain boundary. The model assumes the 3D cavities maintain a fixed equilibrium shape with diameter $2a$ and center-to-center spacing between adjacent cavities $2b$. Note that the finite element implementation of this model does not track individual cavities; the diameter and spacing variables reflect average values at a given integration point. Cavity nucleation decreases the cavity spacing (and increases the cavity density). Cavity growth increases the cavity size.

Several mechanisms contribute to the formation of grain boundary cavities during sustained loading at high temperatures. These include particle cracking and/or debonding, triple point stress

concentrations, and grain slip band dislocation pileup at grain boundaries [11]. However, direct observation and quantification of cavity nucleation is challenging and thus the specific mechanisms and rates of nucleation remain uncertain. Dyson [15] reports that cavity nucleation is a continuous process during creep. Dyson further indicates that the rate of nucleation is controlled primarily by strain rates in adjacent grains. Lim [16] asserts that grain boundary sliding does not contribute to nucleation in a significant way and that nucleation begins during secondary creep such that there is a threshold to the onset of nucleation. Wu and Sandstrom [17] compare several sets of experimental observations and models for cavity nucleation in low-alloy power plant steels. For most cases, the cavity density varies linearly with the creep strain, with the slope dependent on the material and testing conditions.

The nucleation model in the current implementation of grain boundary cavitation, stems from the work of Needleman and Rice [86] and Sham and Needleman [87] and the model of van der Giessen and Tvergaard, as described in [18]. The van der Giessen and Tvergaard model provides continuous nucleation that begins after a stress-strain threshold is met. A rate equation evolves the cavity density N , (e.g., cavities/mm²); the nucleation rate is proportional to the creep strain rate and, optionally, the grain boundary normal traction (to the power β). Table 2-3 presents the governing cavity density rate equation (in terms of the inverse cavity spacing evolution rate, $\dot{b}$) and associated threshold and cavity spacing relationships.

Once nucleated, cavities grow by a combination of diffusion and creep. Table 2-4 presents the traction-separation rate constitutive equations. The coupled diffusional and creep contributions drives the cavity volumetric growth rate, $\dot{V}$, based on the interface normal traction, T_n . The creep contribution considers the stress triaxiality (σ_m / σ_e) and effective creep strain rate ($\dot{\epsilon}_e^C$) in the adjacent grains. This requires a *nonlocal* enhancement to the finite element framework to provide the cohesive elements integration points with stress and strain information from the adjacent solid elements. Dodds *et al.* [12] provide the implementation details for this nonlocal procedure.

Key aspects of the cavity growth model are summarized below.

- Grain boundary sliding does not explicitly contribute to the cavity growth and nucleation equations. Sliding displacements indirectly impact cavity growth by introducing geometric effects (e.g. triple points) that elevate nearby grain stresses, creep rates and the normal tractions acting on grain boundaries.
- The rate equations for volumetric growth, $\dot{V}$, reflect fits to finite element results for models containing discrete voids embedded in a creeping solid over a wide range of triaxialities and porosities $(a/b)^2$, see van der Giessen *et al.* [19,4,5,6,7,8,9,10,13].
- The volume growth rate expressions assume the creep response in the grains has an power law relationship between the stress and strain rate; $\dot{\epsilon}_e \propto \sigma_e^n$. The creep exponent, n , explicitly appears in the $\dot{V}$ equations. The Norton-Bailey (Section 2.1.3) material model requires this exponent as input. The crystal plasticity model computes an equivalent value of n that changes continuously over the loading history. The *nonlocal* feature passes n from the solid elements to the interface elements.

- The q -function has a modification [12] that accelerates the growth rate once the areal porosity $(a/b)^2$ exceeds 0.25. This simulates the interaction and coalescence of adjacent cavities. The unmodified model allows tractions normal to the grain boundary to exist at porosity levels well beyond those measured experimentally near fractured surfaces.
- Under reversed, compressive loading, cavities may reduce in size to the limiting initial value a_0 .

Table 2-1. Variables for cavity nucleation and growth models

Symbol	Description	Units
a	Current cavity radius	mm
b	½ of current center-to-center cavity spacing	mm
$\dot{\delta}$	GB opening displacement rate	$\text{mm} \cdot \text{h}^{-1}$
$\dot{\epsilon}_e^c$	Nonlocal equivalent creep rate	h^{-1}
ϵ_e^c	Accumulated equivalent creep strain (nonlocal)	dimensionless
L	Rice creep-diffusion interaction length	mm
N	Current cavity number density (per unit area)	$\text{cavities} \cdot \text{mm}^{-2}$
S	Non-dimensional stress-strain measure	dimensionless
σ_e	Nonlocal equivalent (von Mises) stress	MPa
σ_m	Nonlocal mean stress	MPa
T_n	Normal traction acting on GB	MPa
$\dot{V}$	Cavity volumetric growth rate	$\text{mm}^3 \cdot \text{h}^{-1}$

Table 2-2: Constants for cavity nucleation and growth models

Symbol	Description	Units
β	Traction exponent	dimensionless
B	Power-law creep, creep coefficient	$\text{MPa}^{-n} \cdot \text{h}^{-1}$
D	Grain boundary diffusion coefficient	$\text{MPa}^{-1} \cdot \text{h}^{-1} \cdot \text{mm}^3$
F_N	Nucleation rate constant	$\text{cavities} \cdot \text{mm}^{-2}$
m	Parameter equal to +1 for tensile stressing, and -1 for compressive stressing	dimensionless
n	Power-law creep, stress exponent	dimensionless
N_I	Initial cavity number density	$\text{cavities} \cdot \text{mm}^{-2}$
$N_{\max}$	Maximum value of the cavity number density	$\text{cavities} \cdot \text{mm}^{-2}$
ψ	Equilibrium cavity tip half-angle ($\sim 70^\circ$)	radians
Σ_0	Traction normalization parameter	MPa
S_{thr}	Threshold value of S for nucleation onset	dimensionless

Table 2-3. Rate equations for cavity nucleation model

$\dot{N} = F_N \left(\frac{T_n}{\Sigma_0} \right)^\beta \dot{\epsilon}_e^C$
Nucleation occurs when $S > S_{\text{thr}}$ and $N < N_{\text{max}}$
$S = \begin{cases} \left(\frac{T_n}{\Sigma_n} \right)^\beta \dot{\epsilon}_e^C, & \text{when } T_n > 0 \\ 0, & \text{otherwise} \end{cases}$
$S_{\text{thr}} \equiv \frac{N_I}{F_N}$
$N_I = \frac{1}{\pi b_0^2}$
$b = \frac{1}{\sqrt{\pi N}}$

Table 2-4. Traction-separation rate constitutive equations

$\dot{\delta} = \frac{\dot{V}}{\pi b^2}$
$\dot{a} = \frac{\dot{V}}{4\pi h(\psi) a^2}$
$\dot{V} = \begin{cases} \dot{V}_L, & \text{if } \dot{V}_L \geq \dot{V}_H \\ \dot{V}_H, & \text{if } \dot{V}_L < \dot{V}_H \end{cases}$
$\dot{V}_L = \dot{V}_L^{(1)} + \dot{V}_L^{(2)}$ $\dot{V}_L^{(1)} = 8\pi D \frac{T_n}{q(f_L)}, \quad f_L = \max\left(\frac{a^2}{(a+1.5L)^2}, \frac{a^2}{b^2}\right), \quad L \equiv \left(\frac{D\sigma_e}{\dot{\epsilon}_e^C}\right)^{1/3}$ $\dot{V}_L^{(2)} = \begin{cases} \dot{\epsilon}_e^C a^3 2\pi h(\psi) m \left\{ \alpha_n \left \frac{\sigma_m}{\sigma_e} \right + \beta_n(m) \right\}^n & \text{if } \left \frac{\sigma_m}{\sigma_e} \right \geq 1 \\ \dot{\epsilon}_e^C a^3 2\pi h(\psi) \left\{ \alpha_n + \beta_n(m) \right\}^n \frac{\sigma_m}{\sigma_e} & \text{if } \left \frac{\sigma_m}{\sigma_e} \right < 1 \end{cases}$
$\dot{V}_H = \dot{V}_H^{(1)} + \dot{V}_H^{(2)}, \quad \dot{V}_H^{(1)} = 8\pi D \frac{T_n}{q(f_H)}, \quad f_H = \frac{a^2}{b^2}$ $\dot{V}_H^{(2)} = \begin{cases} \dot{\epsilon}_e^C a^3 2\pi h(\psi) m \left\{ \frac{1}{1 - (0.87a/b)^{3/n}} \left[\alpha_n \left \frac{\sigma_m}{\sigma_e} \right + \frac{m}{n} \right] \right\}^n & \text{if } \left \frac{\sigma_m}{\sigma_e} \right \geq 1 \\ \dot{\epsilon}_e^C a^3 2\pi h(\psi) \left\{ \frac{1}{1 - (0.87a/b)^{3/n}} \left[\alpha_n + \frac{m}{n} \right] \right\}^n \frac{\sigma_m}{\sigma_e} & \text{if } \left \frac{\sigma_m}{\sigma_e} \right < 1 \end{cases}$
$m = \text{sgn}(\sigma_m), \quad \alpha_n = \frac{3}{2n}, \quad \beta_n(m) = \frac{(n-1)[n+g(m)]}{n^2}$ $g(1) = \ln 3 - \frac{2}{3} \approx 0.4319, \quad g(-1) = \frac{2\pi}{9\sqrt{3}} \approx 0.4031$
$h(\psi) = \left(\frac{1}{1 + \cos \psi} - \frac{\cos \psi}{2} \right) \frac{1}{\sin \psi}$ $q(f_L) \equiv \left(2 \ln \left(\frac{1}{f_L} \right) - (1 - f_L)(3 - f_L) \right)$ $D = \frac{\Omega \delta D_b}{kT} = \frac{\Omega \delta D_{b0} \exp(-Q/RT)}{kT} = \text{material constant}$

2.1.2 Viscous sliding

Table 2-5 presents the rate equations that govern the simple viscous sliding model, with parameters defined in Table 2-6. This implementation extends Ashby's model [20] to 3D by considering shear displacement and tractions on two orthogonal in-plane directions (noted as 1 and 2 in the nomenclature) at each integration point. There is a single material parameter, the viscosity of an uncavitated grain boundary, η_0 , that quantifies the resistance of the grain boundary to sliding deformation. The user may turn on a feature that degrades the effective viscosity as cavities develop and grow. There are no additional user parameters beyond a flag to turn this degradation off and on. When on, the viscosity decreases linearly from η_0 to zero after the porosity reaches 0.25 (i.e., $(a/b = 0.5)$).

Table 2-5. Rate equations for grain boundary sliding model.

$T_{s1} = \eta_b \dot{\Delta}_{s1}$
$T_{s2} = \eta_b \dot{\Delta}_{s2}$
$\eta_b = f_{sd} \eta_0, \quad f_{sd} = f_{sd}(a/b)$

Table 2-6. Nomenclature for grain boundary sliding model and physical units.

Symbol	Description	Units
T_{s1}	Shear traction in the 1-direction	MPa
$\dot{\Delta}_{s1}$	Relative slip rate in the 1-direction	$\text{mm} \cdot \text{h}^{-1}$
T_{s2}	Shear traction in the 2-direction	MPa
$\dot{\Delta}_{s2}$	Relative slip rate in the 1-direction	$\text{mm} \cdot \text{h}^{-1}$
η_b	Viscosity function	$\text{MPa} \cdot \text{h} \cdot \text{mm}^{-1}$
f_{sd}	Viscosity parameter having range from zero to one	dimensionless
η_0	Reference viscosity	$\text{MPa} \cdot \text{h} \cdot \text{mm}^{-1}$
$(a/b)_{\text{onset}}$	Onset values of a/b for viscosity reduction	dimensionless

2.1.3 Norton-Bailey model

The Norton-Bailey model is a simple power-law relationship between stress and the creep strain rate. Table 2-7 and 2-8 list the governing rate equations and nomenclature used for the material properties. The implementation superposes the creep and elastic strain rates; the model requires the typical isotropic elasticity constants and two additional parameters; the creep exponent and creep coefficient. The exponent, n , is generally taken as 5 to represent creep controlled by

dislocation climb/glide and the creep coefficient, B , has representative values of $10^{-15} \rightarrow 10^{-18}$ $\text{MPa}^{-n} \cdot \text{h}^{-1}$. Reference [12] provides implementation details.

Table 2-7. Norton-Bailey constitutive equations for grains

$\dot{\epsilon}_{ij} = \dot{\epsilon}_{ij}^e + \dot{\epsilon}_{ij}^C + \dot{\epsilon}_{ij}^\theta$
$\dot{\epsilon}_{ij}^e = \frac{1+\nu}{E} \dot{\sigma}_{ij} - \frac{\nu}{E} \dot{\sigma}_{kk} \delta_{ij}$
$\dot{\epsilon}_{ij}^C = \frac{3}{2} B \sigma_e^n \frac{s_{ij}}{\sigma_e},$
$\sigma_e = \sqrt{\frac{3}{2} s_{ij} s_{ij}}$
$\dot{\epsilon}_e^C = \sqrt{\frac{2}{3} \dot{\epsilon}_{ij}^C \dot{\epsilon}_{ij}^C}$
$\dot{\epsilon}_{ij}^\theta = \alpha_{ij} \dot{\theta}$

Table 2-8. Norton-Bailey nomenclature and physical units

Property	Description	Units
E	Grain Young's modulus	MPa
ν	Grain Poisson ratio	dimensionless
B	Grain creep coefficient	$\text{MPa}^{-n} \cdot \text{h}^{-1}$
n	Grain creep exponent	dimensionless
σ_e	Equivalent (von Mises) stress	MPa
$\dot{\epsilon}_e^C$	Equivalent creep rate	h^{-1}
$\dot{\sigma}_{ij}$	Stress rates	$\text{MPa} \cdot \text{h}^{-1}$
$\dot{\epsilon}_{ij}$	Total strain rates	h^{-1}
$\dot{\epsilon}_{ij}^e$	Elastic strain rates	h^{-1}
$\dot{\epsilon}_{ij}^C$	Creep strain rates	h^{-1}
s_{ij}	Deviatoric stresses	MPa
$\dot{\epsilon}_{ij}^\theta$	Thermal strain rate	h^{-1}
α_{ij}	Thermal expansion coefficients	$^{\circ}\text{C}^{-1}$
$\dot{\theta}$	Temperature rate	$^{\circ}\text{C/s}$

2.1.4 RVE model

The modeling approach is based on a *RVE* (*representative volume element*) – a volume of material comprised of a sufficient number of randomly sized and shaped grains to represent the heterogeneous microstructure and nonlinear response of the material of interest. Figure 2-2 presents the RVE, or unit cell, employed for all of the simulations in the current chapter.

The cubic domain consists of 100 3D cells that represent prior austenite grains. This geometry is constructed by Voronoi tessellation via the open source Neper software [21]. Neper also meshes the domain with second-order tetrahedral elements. Truster's open source DEIPprogram [22] then inserts 2D 12-node interface cohesive elements between the grains to define the 467 grain boundaries. Additional details of these programs and their use in generating the RVE are found in [12].

The $X = 0.0$ mm, $Y = 0.0$ mm, and $Z = 0.0$ mm planes have symmetry boundary conditions. The $X = 0.2$ mm, $Y = 0.2$ mm, and $Z = 0.2$ mm planes have multipoint constraints to enforce uniform normal displacement during the simulation while leaving the in-plane displacements unconstrained.

The creep simulations in this chapter all employ a load-hold strategy. An applied load on a single node on the $Y = 0.2$ mm plane imposes (via the multi-point constraints) a uniform applied uniaxial stress on this plane. The use of an applied force allows the magnitude of the stress to change as the cross-sectional area changes in geometrically nonlinear simulations. The loading history ramps the applied force from 0 to the maximum value (simulation dependent, generally to provide an applied stress of 60-200 MPa) over 0.1 h. This traction is then held at this level for the remainder of the simulation (up to 10^6 h, depending on the traction magnitude).

The primary results of interest are the so-called cell strain and cell strain rate. The cell strain is taken as the displacement of the loaded surface ($Y = 0.2$ mm) in the loading direction (Y) divided by the cell height (0.2 mm). This strain includes the elastic, creep, and viscous response of the grains and grains boundaries. The cell strain rate is simply the time rate of change of the cell strain. The simulations also track internal variables to monitor the progress of grain boundary nucleation and cavitation. Physical units employed in all the simulations are: MPa, h, mm, N. For the simulations employing the Norton-Bailey model, material properties assigned to the grains are: $E = 150,000$ MPa, $\nu = 0.285$, $n = 5$, $B = 1.0 \times 10^{-16}$ MPa $^{-n} \cdot \text{h}^{-1}$.

Extensive previous studies with this RVE have ascertained the following:

1. Cell response is independent of the loading direction (X , Y , or Z)
2. The 100 grain model provides a representative response for this grain size and shape distribution, i.e., an 800-grain model with the same characteristics provide essentially the same response to creep loading.

3. Cell strains and strain rates, especially during secondary and tertiary creep, are generally independent of the time step size (other than the effect of step size on global numerical convergence).
4. The grain size and shape distributions are approximately representative of Grade 91 PAGs.

2.2 Numerical Improvements

Enhancements to the grain boundary cavitation model since the previous update [12] focus on algorithmic improvements. The main issues are summarized below, with additional details on the problems, and solutions, provided by the following subsections.

- For some simulations, the global Newton iterations failed to converge for some steps during initial loading regardless of timestep size reductions and convergence tolerance relaxations. Minor adjustments to the code logic greatly improve these convergence issues. With judicious time step sizes and allowing adaptive step size refinement, simulations now meet reasonable convergence tolerances for every step until well into the tertiary creep phase and the development of full grain boundary failures. Section 2.2.1.1 outlines the numerical procedure/logic for the normal traction/separation response of the grain boundary cohesive model.
- Nonrealistic oscillations and noise in the cell strain rate response occurred at early-to-moderate timesteps for some simulations both with cavitation and without cavitation. Figure 2-3 demonstrates these issues, for a cell simulation. The yellow spikes occur at time step changes if the general grain boundary response in the cell is linear (no active cavitation) and the linear stiffness magnitude is calculated based on continuity at the onset of cavitation. Previous work, *e.g.*, [12] use this so-called K_{lin}^{alg} approach (see Section 2.2.1.2.) These strain rate spikes along with traction-related numerical problems (see next bullet) motivate the change to a user-defined linear stiffness, K_{lin}^{user} . While this constant linear stiffness does indeed resolve some computational concerns, the magnitude can have a strong influence on the early response of the cell, including noise level. In the figure, note that the local noise (small timescale fluctuations about a mean) increase as K_{lin}^{user} increases. The higher stiffness values also lead to a non-physical oscillation on a hundreds-of-hours timescale. Section 2.2.1.2 discusses the linear stiffness implementation and values in more detail.
- Oscillations and high magnitudes in grain boundary normal tractions vary with the normal stiffness and can produce undesired nucleation and cavitation rates. The nature and cause of these normal traction issues are discussed further in Sections 2.2.1.3 and (Chapter 4). These problems are mitigated by (1) limiting the linear normal stiffness (2) setting the shear stiffness and normal stiffness magnitudes to similar orders of magnitude and (3) us-

ing resolved tractions from the adjacent solid elements to control nucleation and cavitation rather than the interface element normal tractions.

- The RVE simulations typically experience global convergence failure before reaching strain levels attainable in physical experiments. Modifications to help drive effective cavity coalescence improve the tertiary response trace somewhat. However, examination of the grain boundary failure progression does indicate that the cell response is well into the tertiary creep phase before numerical failure, and further progress along the curve actually would provide relatively little further information about failure times and mechanisms.

2.2.1.1 Normal traction/separation response flow diagrams

The normal traction/separation response of the grain boundary cohesive model involves as much logic and branching as floating point operations. The current state (open, closed, neutral) and state change (opening vs. closing) of the interface, nucleation activity (threshold not met, active nucleation, maximum cavity density reached), and cavitation progression (not yet nucleated, active cavitation, cavity coalescence) all affect the normal $T - \delta$ response during a time step.

Figure 2-4 illustrates the logic sequence to determine if the global solution iteration requires a full cavitation update or just a linear update at a given interface element integration point. Figure 2-5 provides the logical structure of a cavitation-based update, although the calculations may indicate that the response of the integration is actually linear (no cavitation) during the global iteration. Figure 2-6 shows the simple steps in a linear update; for which the only branching is based on providing a stiffer response to prevent interpenetration of interface elements under compression.

2.2.1.2 Grain boundary normal stiffness

The grain boundary cavitation model defines the relationship between the normal traction and the normal opening rate. Outside of a finite element framework, this cavitation-based relationship is sufficient to describe the behavior of a grain boundary. Before nucleation, there is no normal opening and after nucleation the cavitation-based equations (Section 2.1.1) dictate the normal opening/traction response. In the finite element framework, the grain boundary cohesive elements must have a stiffness that defines the normal traction-opening response at all times, e.g. even before cavity nucleation. Ideally, this stiffness will be large enough that grain boundary opening before cavitation is essentially zero, and certainly much smaller than other deformations (i.e., the grain boundary response during cavitation and strain in the grains). However, an overly large normal stiffness leads to numerical inaccuracies and convergence problems.

The approach, until recently, was to compute the linear stiffness of the grain boundary so that the stiffness would be continuous at the onset of cavitation. The stiffness of the cavitation response is given Eqn (2.1)

$$\frac{dT_n}{d\delta} = K = \frac{b^2 q(a,b)}{4D \cdot dt} \quad (2.1)$$

Thus the algorithmic linear stiffness is

$$K_{lin}^{alg} = \frac{b_0^2 q(a_0, b_0)}{4D \cdot dt} \quad (2.2)$$

For typical (for these Grade 91 studies) parameter values of $a_0 = 50$ nm, $b_0 = 60$ μ m, $D = 8 \times 10^{-15}$ MPa $^{-1} \cdot$ h $^{-1} \cdot$ mm 3 , K_{lin}^{alg} ranges from 10^{14} MPa/mm when $dt = 0.01$ h to 10^{11} MPa/mm when $dt = 10$ h.

Note the appearance of the time step size, dt , in K_{lin}^{alg} . Figure 2-3 reveals that this can lead to the spikes in the cell strain rate. While these spikes are indeed non-physical and disconcerting, there is a more insidious problem with using this computed value for the linear stiffness.

The top left contour plot in Figure 2-7 reveals the distinct “checkerboard” traction oscillation pattern and high traction magnitudes that can develop with high interface normal stiffness ($K_{lin}^{user} = 10^{10}$ MPa/mm). This is essentially a linear elastic response; nucleation and cavitation are turned off and the time scale prevents significant creep strain in the grains (Norton-Bailey model). Elements with tensile tractions of order 2,000 MPa are adjacent to elements with compressive tractions of the same magnitude. The applied stress is only 100 MPa so the high traction magnitude (20x applied) and oscillating directions (tensile vs compressive) is indicative of computational inaccuracies.

A more moderate interface normal stiffness ($K_{lin}^{user} = 10^8$ MPa/mm) reduces the traction oscillation and nearly halves the maximum traction magnitude, as shown in the upper right contour plot. The tractions on interfaces normal to the loading direction generally have tensile tractions with magnitudes typically below 500 MPa. Nevertheless, the maximum traction magnitudes (1,500 MPa) are still larger than realistic.

A lower interface normal stiffness ($K_{lin}^{user} = 10^6$ MPa/mm) essentially eliminates the checkerboard effect and brings traction magnitudes back down to reasonable levels. However, a stiffness this low leads to large interface openings that dominate the cell response. The line plot in the lower right shows the displacement at the top of the cell during the loading ramp for the three different interface stiffnesses. For a linear elastic cell with no interfaces and the same grain elastic modulus, the cell displacement for 100 MPa applied stress is 0.133 mm. Interface opening increases the total cell displacement above this no-interface elastic baseline. The high interface stiffness case allows displacements 1.2 times higher than the no-interface baseline. The intermediate stiffness case, with a large improvement in traction behavior, only moderately increases the additional cell displacement (1.6 x baseline). The low interface stiffness however dramatically increases the net cell response; displacements are seven times greater than without interfaces. For this set of material, geometric, and loading parameters, a K_{lin}^{user} of order 10^7 - 10^8 MPa/mm provides a reasonable balance between artificial interface opening and numerical stability.

The deformations and stresses discussed above are for simulations with very low sliding viscosity ($\eta_b = 100$ MPa $\cdot$ h $\cdot$ mm $^{-1}$). This essentially free sliding condition represents worst-case conditions; increasing the sliding resistance decreases opening deformation and reducing traction

oscillations. With $\eta_b = 10^6 \text{ MPa} \cdot \text{h} \cdot \text{mm}^{-1}$ and $K_{lin}^{user} = 10^6 \text{ MPa/mm}$, the cell displacement at 100 MPa is 0.3 mm; still more than double the interface-free value but much lower than with free sliding.

The results correspond to a cell model with the same grain structure and loading as described in Section 2.1.4 but with the finer mesh density. There are 125,000 nodes and 69,000 solid elements in the refinement model compared to 25,000 nodes and 10,000 solid elements in the standard model. The standard density mesh exhibits similar traction checkboard patterns and magnitudes.

As discussed above, the use of a moderate linear stiffness magnitude to mitigate traction oscillations does introduce additional strain in the cell that can be viewed as a linear-elastic opening of the grain boundaries. Figure 2-8 considers the magnitude of this elastic opening compared to other sources of strain in the RVE. Cavitation is turned off so that all opening response is governed by the linear stiffness. The shown curves represent two separate simulations with all inputs equal except for the linear opening stiffness. The dashed lines correspond to $K_{lin}^{user} = 10^7 \text{ MPa/mm}$; the solid lines to 10^{10} MPa/mm . During initial loading (up to $t = 0.1 \text{ s}$), the total strain rate is of order 10^{-2} h^{-1} for both simulations, but slightly higher for the $K_{lin}^{user} = 10^7 \text{ MPa/mm}$ simulation. The normal opening rate during initial load is, as expected, 3 orders of magnitude smaller for the simulation with the 10^3 times higher stiffness, but because the strain rate in the grain is significantly higher during load, K_{lin}^{user} has only a small influence on the total cell response. However, after initial loading, the grain strain rate is purely creep based and drops precipitously. The K_{lin}^{user} term now has a strong effect on the overall strain rate, with total strain rates differing by a factor of 5 at 100 h. The opening stiffness also affects the strain rate from grain boundary sliding. As noted in previous studies, grain boundary sliding and opening are geometrically coupled by the tortuous grain boundaries; opening cannot occur if sliding is prevented on adjacent but perpendicular boundaries [12]. Conversely, higher sliding rates occur when greater normal opening develops stress concentrations at triple points. The grain strain rate differentiates for $t > 1 \text{ h}$; the lower grain boundary stiffness increases the grain strain rate, due to the increased stress concentrations from more grain boundary deformation.

With the pre-nucleation normal response of the grain boundary now set by a user-defined parameter, rather than a parameter based on stiffness continuity, the onset of nucleation can lead to anomalies. Figure 2-9 (top plot) presents the strain rate, by mechanism, for two simulations with equal K_{lin} values. One simulation (dashed lines) is the purely linear grain boundary normal response (no cavitation), as in the previous figure but out to longer times. The dashed-dotted lines correspond to simulations for which the normal response is linear until nucleation and cavitation-based thereafter. The creep strain rates are coincident for these two simulations until nucleation begins in some elements, at about 0.6 h. Once nucleation occurs, the grain boundary opening rate drops rapidly and actually becomes negative. The negative values cannot be shown on a log scale but are indicated by the lack of green dash-dot curve from $t = 1 \text{ h} - 12 \text{ h}$. During this time period the grain boundaries are adjusting to the much stiffer early cavitation response compared to the linear stiffness. However, as the porosity increases, the cavitation model strain rates catches up to and then surpasses the linear model.

The top plot represents the two bounding cases; either the response is purely linear ($T_n = K_{lin}\delta$, dashed lines in plot) during the simulation or the response is linear until nucleation and cavitation (as defined by equations in Table 2-4, dashed-dotted lines in plot) after the nucleation threshold is met. The lower plot in the figure adds curves for a model that maintains the linear response through the simulation and superposes the cavitation response after nucleation. The new curves initially coincide with the linear-only curves but transition to follow the cavitation curves up through failure. The major benefits of this superposition of opening mechanisms are (1) improved numerical convergence due to the continuity at the onset of nucleation and (2) elimination of the suspect negative grain boundary strain rates that suppress the total strain rate during this time frame. Maintaining the linear response through superposition does not significantly influence the tertiary response and time to failure. This is a good indication that using a moderate linear stiffness to improve numerical issues does not alter time-to-failure responses in an appreciable way.

2.2.1.3 Interface normal tractions

Section 2.2.1.2 introduces the occurrence of unstable normal tractions in the grain boundary elements that manifest as high magnitudes (up to 20 times higher than the applied stress) and oscillating signs between adjacent interface elements. These problems are particularly severe early in a simulation and occur with or without cavitation (*i.e.*, it is an element issue, not a cohesive model artifact). Judicious selection of the normal direction linear stiffness and sliding viscosity can significantly reduce the severity of this poor traction behavior. See Chapter 4 for further details.

The erroneously high tractions early in a simulation have deleterious effects on the nucleation and growth of cavities. The normal traction, calculated directly from the interface opening, δ , for the current iteration, explicitly appears in both the cavity growth rate and possibly the nucleation rate (depending on user input parameter β). A computed tensile normal traction that is an order of magnitude or more higher than it should be artificially accelerates the nucleation, growth, and even coalescence of grain boundary cavities. Computed high magnitude compressive normal traction erroneously close existing cavities back to their initial size, possibly in a single time step. The spatial and temporal oscillation in these extreme traction values lead to global convergence problems with extremely stiff traction/separation response (small cavities, interface compression) alternating with very soft response (large and/or closely spaced cavities).

The grain solid elements stress fields are far more stable than the interface element tractions. The *nonlocal* character of the cavity growth model already requires the stress fields from the adjacent solid elements. The current framework in WARP3D passes the solid stress fields from the previous converged time step into the cohesive model update for the current global iteration. It is a simple extension to resolve the solid element stress fields to compute the traction in the interface normal direction. The cohesive model computes and then averages this effective normal traction from the solid elements on both sides of an interface element. In a numerically well-behaved scenario, this T_n^{solid} value and the interface cohesive model traction are equivalent. In practice there may be a large disparity due to the aforementioned problems with the interface normal tractions. The T_n^{solid} value now drives the cavity size and spacing updates in the code.

This greatly improves the global convergence early in the simulations and eliminates erratic cavity nucleation and growth.

Figure 2-10 compares the normal tractions from resolved solid element stresses to normal tractions from the interface opening (δ). All six contour plots correspond to the same time point (end of ten step, one hour ramp to 100 MPa applied stress on $Y = 0.2$ mm RVE surface). The contour limits (-200 to 200 MPa) are the same in the six plots to emphasize the differences due to the interface cohesive model linear stiffness (10^{12} to 10^6 MPa/mm) and method of calculating the normal traction. The displacements are multiplied by a factor of 50 in all plots; this highlights the effect of the linear stiffness on the cell deformation. As noted in the line plot of Figure 2-7, $K_{lin} = 10^6$ MPa/mm allows much more grain boundary opening, and thus total cell deformation than $K_{lin} = 10^8$ MPa/mm. A further increase in K_{lin} to 10^{12} MPa/mm reduces the cell deformation but much less dramatically. Note that these simulations all use a very low sliding viscosity ($\eta_b = 100$ MPa $\cdot$ h $\cdot$ mm⁻¹) that essentially allows free sliding. This can lead to much larger grain boundary interface deformation than when the viscosity is high and the lack of sliding geometrically restricts interface opening. Thus, the effect of K_{lin} on the deformation shown here is extreme.

When the interface tractions come from resolved solid element stresses, the maximum ratio of normal traction magnitude to applied stress is generally less than 2.0 and always less than 4.0, for the range of linear stiffnesses used. Indeed, with $K_{lin} = 10^{12}$ MPa/mm the maximum tensile T_n^{solid} is 202 MPa and the maximum compressive T_n^{solid} is -94 MPa. This is in stark contrast to the traction range based on interface opening (24,000 to -30,000 MPa!), and the contours are smooth (not oscillating element by element). Normal tractions are generally tensile on interfaces perpendicular to the loading direction, neutral on interfaces parallel to the loading direction, and compressive at triple points, as expected.

With a decrease in the interface linear stiffness to 10^8 MPa/mm, the resolved solid element stress based interface tractions maintain the same well-behaved appearance as with the higher stiffness. The tractions are somewhat larger however (general between 200 and -200 MPa but with maximum magnitudes reaching 380 MPa in tension and 260 MPa in compression). This is because the softer response of the interfaces allows more local deformation and thus higher stress concentrations. The range of interface opening based normal tractions (1,300 to -1,500 MPa) is still nearly an order of magnitude higher than for the resolved solid stress tractions for this same linear stiffness.

Reducing K_{lin} to 10^6 MPa/mm leads to more widespread high-magnitude tractions (from resolved solid stresses) although the maximum tension is similar to the $K_{lin} = 10^8$ MPa/mm case (380 MPa) and the maximum compression somewhat lower (-190 MPa). The solid-stress based normal tractions and interface opening based normal tractions are very similar in both magnitude and distribution for this low interface normal stiffness case. However, as K_{lin} in the range of 10^7 - 10^8 MPa/mm keep interface strains at least an order of magnitude smaller than the elastic response of the grains, the use of T_n^{solid} along with K_{lin} above 10^6 MPa/mm achieves a reasonable balance between competing numerical issues.

2.2.1.4 Failure during tertiary creep

The simulations with cavitation reproduce the onset of tertiary creep with an upturn in the strain rate approaching a vertical asymptote indicative of cell failure. This is a numerically challenging regime however as the stiffness of cohesive element integration points undergoing cavity coalescence goes to zero. The global Newton iterations typically show oscillatory behavior in which the successive iterations bounce between two small residual values. As the failure progresses, further numerical progress (additional time steps) may require relaxation of the convergence tolerance. Nevertheless, the simulations generally progress far enough up the failure response that the time-to-failure can be quantified with confidence. Indeed the asymptotic character of the strain rate during tertiary creep means little further information would come from tracing the response much further.

One algorithmic change during the current project year did improve numerical performance during tertiary creep. The stiffness of the cavitation response depends on many factors but the largest contribution to the change in the stiffness as cavities grow is the q -function (see Table 2-4). As described in [12], the numerical implementation modifies the base version of the function to (1) force an effective cavity coalescence as the porosity increases and (2) prevent the interface stiffness from getting so low that numerical issues arise. This modification transitions the value of q to a minimum value ($q_{\min}$, set in the source code) as the porosity, $f = (a/b)^2$, reaches 0.49, i.e., $a/b = 0.7$. This is done by substituting a third order Hermitian polynomial (q_{mod}) for the baseline q function (given in Table 2-4) for $f_i < f \leq f_j$ such that $q_{\text{mod}}(f_i) = q(f_i)$, $q'_{\text{mod}}(f_i) = q'(f_i)$, $q_{\text{mod}}(f_j) = q_{\min}$, and $q'_{\text{mod}}(f_j) = 0$. The transition interval is hardcoded to $f_i = 0.25$ and $f_j = 0.49$. The value of $q_{\min}$ is somewhat arbitrary. Previously, $q_{\min}$ was 10^{-3} ; about half the value of the base function at $a/b = 0.9$. This value allowed a swift but graceful failure of simple two-grain tests. However, it may prevent the interface stiffness from reaching a failure state with essentially zero-magnitude normal tractions.

Figure 2-11 examines the effect of $q_{\min}$ on RVE simulations. The only difference between the three sets of results in the figure is the value of $q_{\min}$; ranging from 10^{-3} to 10^{-9} . The cell strain rates and strains are coincident until near the end of the simulations. With $q_{\min} = 10^{-3}$, the global solution procedure fails to converge around 12,800 h with strain rate of $2.2 \times 10^{-5} \text{ h}^{-1}$ and a total cell strain of 6%. A $q_{\min}$ of 10^{-6} allows the simulation to proceed a bit further before numerical failure to 14,500 h with a much greater strain rate ($2.6 \times 10^{-4} \text{ h}^{-1}$) and significantly more cell strain (26%). Another reduction in $q_{\min}$ to 10^{-9} allows the simulation to reach 43% total strain and $5.2 \times 10^{-4} \text{ h}^{-1}$ strain rate with only a small increase in time to 14,800 h. Thus there is an additional 2,000 h on the time-to-failure (14%) by lowering $q_{\min}$ from 10^{-3} to 10^{-9} , but only an additional 300 h (2%) comes from $q_{\min}$ decreasing from 10^{-6} to 10^{-9} . These simulations employ the NB model for the grain response and linear deformation mechanics.

The crystal plasticity model (Chapter 3) vastly increases the computational complexity compared to the simplistic Norton-Bailey model. While details of the interactions between the CP

and grain boundary cavitation model are left for later chapters, this section briefly discusses time-to-failure issues based on the simulations with the CP model.

Figure 2-12 shows strain rate histories for simulations employing the CP model for grain response along with the full cavitation model on the grain boundaries. Parameters are the same for the three simulations except for the applied load (100, 120, and 140 MPa). The figure includes test data at these loads from Kimura *et al.*, [23] to indicate the expected behavior in tertiary creep along with experimentally attainable strain rates. These simulations are representative; Chapter 6 explores parameter calibration and nuances of the interactions between the grain and grain boundary responses.

For the 140 MPa simulation numerical failure occurs at 3,300 h, with 2.4% total strain and 2% area reduction. At this point, seven full grain boundaries (all elements on the boundary) have reach an a/b ratio of at least 0.9. Figure 2-13 (a) shows the cell deformation (5X displacement magnification) at grain stress (in the loading direction, Y) at the last time step. The grain boundary opening is clear and indicates the formation of at least one failure surface extending over most of the cell. While the total cell strain is relatively low (compared to that achieved with some of the Norton-Bailey simulations), cell failure is well underway.

The 120 MPa simulation terminates at 8,200 h with a total strain of 2.1% and two full grain boundaries with $a/b > 0.9$. While this is slightly less strain and grain boundary “failure” than at the termination step for the 140 MPa model, the extent of grain boundary separation is similar. Figure 2-13 (b) presents the cell deformation at the termination step for the 120 MPa simulation; it is nearly indistinguishable from the 140 MPa case.

The extent of the 140 MPa and 120 MPa simulations reflect several adjustments to time step sizes and global convergence tolerances to advance the solution as far as possible (while maintaining reasonable accuracy). The 100 MPa simulation did not undergo these refinements and thus incremental increases in strain rate and total strain may be possible but significant gains without algorithmic changes are unlikely.

Figure 2-14 confirms that the normal tractions in the failing grain boundary elements do indeed go toward zero, as expected. The figure only shows cohesive elements with $a/b > 0.9$. Tensile tractions are less than 10 Pa and compressive traction magnitudes are less than 10 MPa. Invoking an element extinction feature that removes failed elements from the simulation may improve the ability to reach higher cell strains.

2.3 Parameters

The current form of the grain boundary interface-cohesive model provides a flexible framework for describing the normal traction/opening response. The model requires up to eighteen input parameters; six Boolean flags and 12 numerical constants. Each grain boundary may have its own unique set of input parameters. Table 2-9 and Table 2-10 briefly define the required parameters. The typical values presented correspond to the simulation of Grade 91 steel. An overview of the range of normal response is given below, and then the following subsections examine the numerical parameters in more detail.

Figure 2-15 compares the cell response (strain rate history) for several different general grain boundary opening response definitions. The dashed blue line that forms the lower bound repre-

sents the Norton-Bailey model creep response of the grains in uniaxial loading; no elasticity and no grain boundary deformation; $\dot{\epsilon}_c = B\sigma^n$. The solid red line maintains this model for the grains, but with elasticity included; note the much higher strain rate (10^{-2} h^{-1}) during the loading ramp ($t > 0.1 \text{ h}$). The grain boundary opening is linear-elastic (*include cavity growth* = F) and has high resistance to sliding ($\eta_b = 10^{12} \text{ MPa} \cdot \text{h} \cdot \text{mm}^{-1}$). The cell strain rate transitions from the high value during loading to the constant Norton-Bailey creep rate over 1,000 h. Note that both of these bounds are dictated purely by the grain response. The high viscosity prevents not only tangential grain boundary sliding but also geometrically restricts grain boundary normal opening, despite the moderate interface normal stiffness.

The solid green line represents essentially free sliding ($\eta_b = 10^2 \text{ MPa} \cdot \text{h} \cdot \text{mm}^{-1}$). The strain rate during the loading phase doubles relative to the no-sliding case. The strain rate drops several orders of magnitude immediately after the reaching full load (i.e., when $d\sigma_{\text{applied}}/dt$ goes to 0). However, by the end of the simulation at 30,000 h (end of load steps), the strain rate has not reached the grain-only base line. This indicates that grain boundary deformation continues, despite the lack of cavitation.

The blue solid line corresponds to an intermediate sliding viscosity ($\eta_b = 10^6 \text{ MPa} \cdot \text{h} \cdot \text{mm}^{-1}$). This magnitude of sliding viscosity provides the smoothest grain boundary deformation, as explained in Chapter 4. The strain rate during loading is closer to the no-sliding case than the free sliding case while during most of the hold time ($t < 20 \text{ h}$), the cell strain is indistinguishable from the free sliding case. For $0.1 \text{ h} < t < 20 \text{ h}$, the intermediate sliding viscosity case produces a higher cell strain rate than seen with either free sliding or no sliding. This viscosity is not so high as to prevent all grain boundary deformation (as for the no-sliding case) and the allowed normal deformation and proportional tangential tractions lead to higher stress concentrations than for the free sliding case. As the grain boundaries deform, the stress concentrations relax and the system returns to free-sliding conditions.

The magenta dashed line includes cavity growth but not nucleation (*include cavity growth* = T , *include nucleation* = F). From $t = 0$ the cavities may begin to grow (from size a_0) but the cavity density does not change during the simulation. The cell response is indistinguishable from that of the no-cavitation case until $t > 30,000 \text{ h}$. After this time, the cell strain rate begins to accelerate. If the initial cavity size and/or initial cavity density was larger the distinction between cavitation and no-cavitation would be apparent earlier in the simulation.

The final curve in the plot allows cavity nucleation (*include nucleation* = T). The grain boundary normal response is linear-elastic until the cavity nucleation threshold is met. When the threshold is reached at an integration point, the integration point normal response immediately includes the effects of cavities with density N_f and size a_0 . Under sustained tensile loading, cavities nucleate and grow continuously until meeting a bound (maximum cavity density or cavity coalescence). This curve represents the full interface-cohesive response to represent PAGB deformation in Grade 91 steels; tangential sliding, nucleation and growth of cavities when sufficient deformation accumulates in the surrounding material, and continuous cavity nucleation and growth reducing capacity of grain PAGBs to carry tractions leading to local microcrack for-

mation. The set of parameters stated in Figure 2-15 are the baseline of the parameter study presented below; unless otherwise stated these values remain in effect for the rest of the chapter.

Table 2-9: Boolean Input Parameters for Interface-Cohesive Model

Parameter name	Description	Typical Value
degrade shear viscosity	If T , reduces resistance to sliding as cavities coalesce and consume interface. If F , the shear viscosity remains equal to the constant user-input value during the simulation.	T
use VNNT equations	If F , reverts to simpler model for cavity volumetric growth by creep, see [12]. If T , uses the equations in Table 2-4 .	T
modify the q -value	If T , drives cavity coalescence when a porosity of $(a/b)^2 = 0.25$ is reached by transitioning from the q -function in Table 2-4 to a low value (q_{min}). If F , the basic q -function in Table 2-4 is used for all porosities.	T
include nucleation	If F , cavities are present and may grow from beginning of simulation but no new cavities form. If T , cavities nucleate (and then grow) only after a local stress-strain threshold is met.	T
include cavity growth	If F , interface normal response is purely linear-elastic, controlled only by the input linear stiffness. If T , cavity growth may occur, depending on nucleation status.	T
compute T_n from solid elements	If T , the output normal traction for post-processing, is based on the stress fields in adjacent solid elements. This flag does not alter calculations during solution. If F , the output normal traction for post-processing comes from the interface element displacement jumps (opening).	F

Table 2-10: Numerical Input Parameters for Interface-Cohesive Model

Parameter Name	Description	Typical Units	Typical Value (or Range)
a_0	initial cavity radius, a_0	mm	5×10^{-5}
b_0	half initial distance between cavities, b_0	mm	6×10^{-2}
eta_b	sliding viscosity, η_b	MPa · h · mm ⁻¹	10^6
D	Diffusivity, D	MPa ⁻¹ · h ⁻¹ · mm ³	10^{13} to 10^{16}
n	Creep exponent n (only used on 1 st load step, thereafter the adjacent solid elements pass in an effective value)	unitless	5.0
psi_angle (degrees)	Equilibrium cavity tip half-angle, ψ	degrees	75
sigma_0	Traction normalization parameter, Σ_0	MPa	100
F_N / N_I	Nucleation rate (normalized), F_N / N_I	unitless	10^3 to 10^5
N_max / N_I	Maximum cavity density (normalized), N_{max} / N_I	unitless	1 (no change in cavity density) to 10^6 (unlimited cavitation)
nucleation stress exponent	Set nucleation rate dependence on normal traction, β	unitless	0 (nucleation independent of T_n) to 2
compression multiplier	Stiffened response factor to avoid interface interpenetration, m	unitless	10
linear stiffness	Elastic normal traction/separation response (needed for computational stability), K_{lin}	MPa/mm	10^7 - 10^8

2.3.1 Initial cavity radius

An earlier study [12] finds that the initial cavity size, a_0 , has a very modest effect on the time-to-failure for values less than 500 nm. Figure 2-16 confirms this observation for the current form of the cavitation model. Indeed, the strain rate histories are indistinguishable for initial cavity radii of 50 nm and 500 nm (magenta and green curves, top plot). The middle plot in the figure, which shows the average cavity size evolution, demonstrates that the initially smaller cavities grow faster and eventually nearly catch up to the initially larger cavities.

A study of experimental results indicates a reasonable final cavity radius for Grade 91 steel is 2-7 μm . At simulation failure during tertiary creep, the average calculated cavity radius is 1 μm and the maximum cavity radius is 3 μm , which agree well with the experimental findings.

2.3.2 Initial cavity spacing

The grain boundary opening rate is proportional to the square of the cavity spacing; decreasing b by a factor of ten increases the grain boundary opening rate by a factor of 100. The spacing also influences the cavity volumetric growth rate, $\dot{V}$. An earlier examination of the effect of the initial cavity spacing [12] reveals a dramatic effect on the strain rate history. That study did not include nucleation; the cavity spacing remains constant throughout the simulation.

Figure 2-16 demonstrates the strong role the initial cavity spacing plays on the strain rate when nucleation of new cavities is included. Halving the initial cavity spacing from $b_0 = 60 \mu\text{m}$ to $b_0 = 30 \mu\text{m}$ cuts the lifespan from 11,000 h to 4,500 h. The middle plot indicates that the cavity size evolution is essentially independent of the spacing, until cavity coalescence sets in and the growth rate accelerates. The bottom plot shows the evolution of the average cavity spacing. The average spacing is fairly constant for the first few hundred hours, before nucleation is widespread. As more grain boundaries accumulate enough creep strain to nucleate cavities the cell average rate of decrease in cavity spacing becomes linear, as expected based on the evolution equation when the strain rate is constant (for these $\beta = 0$ simulations; i.e., no traction contribution to nucleation).

Changing the initial cavity spacing changes the initial cavity density, N_I , and thus the nucleation rate parameter F_N because the user specifies F_N / N_I . Of course, the F_N / N_I input can be modified to maintain constant F_N for different values of b_0 . This would, however, change the nucleation threshold, N_I / F_N (see Table 2-3). Thus for constant F_N a decrease in the initial cavity spacing (increase in initial cavity density) increases the nucleation threshold (more strain must accumulate before cavities nucleate).

Experimental measurements with Grade 91 steel indicate a center-to-center cavity spacing ($2b$) at failure of 30 to 70 μm , [12]. The simulation with $b_0 = 60 \mu\text{m}$ evolves to an average center-to-center cavity spacing at failure of $2b_{\text{avg}} = 54 \mu\text{m}$, with a minimum (among all integration points) of $2b_{\text{min}} = 7 \mu\text{m}$. The simulation with $b_0 = 30 \mu\text{m}$ leads to smaller final sizes; $2b_{\text{avg}} = 23 \mu\text{m}$ and $2b_{\text{min}} = 2 \mu\text{m}$. The computed average spacings are thus reasonable and indeed

the experiment values are based on average number of cavities in a viewing area and not cavity-by-cavity measurements.

2.3.3 *Sliding viscosity*

Figure 2-15 and the associated discussion at the beginning of Section 2.3 compare the cell strain rate history for three different values of the sliding viscosity, in the absence of grain boundary cavitation. Figure 2-17 examines the decomposition of the total strain rate into contributions from grain boundary opening, grain boundary sliding and grain deformation. The no-sliding case in the top plot actually has some sliding because the viscosity is not infinite though it is at least two orders of magnitude smaller than the grain response. The total strain rate is set by the grain strain rate during active loading and up through $t = 1$ h and for $t > 20,000$ h. At intermediate times, the opening deformation controls the total strain rate but with sliding suppressed the opening rate diminishes because of geometric locking. This locking prevents stress concentrations and thus grain strain rate is that of a continuum Norton-Bailey response.

The free sliding case (middle plot) exhibits a much larger sliding contribution to the total strain rate than the no-sliding simulation. Cell strain from sliding is actually somewhat greater than all other components for $t < 50$ h. Both sliding and opening decrease as stress concentrations are relieved by the deformation, without cavitation to drive continued interface deformation. The grain deformation rate also decreases with time, but more slowly than the grain boundary deformation mechanisms.

For the intermediate viscosity case, the bottom figure reveals sliding drives the total cell strain rate early in the simulation. The sliding deformation and shear tractions also increase grain boundary opening and grain deformation rates during this transient phase. Ultimately though the opening deformation goes to zero (no cavitation) and grain boundary sliding and grain deformation decrease too, albeit slowly. As discussed in Chapter 4, intermediate viscosity values, like the $10^6 \text{ MPa} \cdot \text{h} \cdot \text{mm}^{-1}$ used here, minimize numerical problems with the interface elements and the increase in the early strain rate, relative to a free-sliding model, improves the model's ability to fit the primary creep phase to experimental data.

2.3.4 *Diffusivity*

A study of experimental measurements, see [12], concludes that the diffusivity may range from 10^{-13} to $10^{-16} \text{ MPa}^{-1} \cdot \text{h}^{-1} \cdot \text{mm}^3$ for Grade 91 steels, with minor changes in Cr content causing relatively large changes in diffusivity. Figure 2-18 investigates the effect of the diffusivity on the cell strain rate, cavity growth and cavity density. The magenta dashed curves and blue solid curves represent an order of magnitude change in the diffusivity. The magnitude of the diffusivity does not affect the cell strain rate until about $t = 100$ h, after which the higher diffusivity drives earlier tertiary creep and failure. Faster cavity growth, as measured by the maximum cavity size among all integration points (middle plot), actually begins quite early ($t = 2$ h). The maximum cavity size in the higher diffusivity simulation is generally twice that of the smaller diffusivity case. The evolution of the maximum cavity density (bottom plot) does not differentiate until 100 h, when the higher diffusivity case actually falls behind the lower diffusivity case. However, after 3,000 h the higher diffusivity case sees its cavity density increases rapidly during the tertiary

creep phase. This is a challenging parameter to calibrate; there is wide range in values from experimental data and yet the model is quite sensitive to these order-of-magnitude changes.

2.3.5 Cavity nucleation rate and threshold

The nucleation threshold is the inverse of the input F_N / N_I parameter; higher F_N / N_I values reduce the strain (and/or normal traction, depending on nucleation exponent β) at which cavity nucleation begins. Higher values of F_N / N_I also increase the rate of nucleation. Figure 2-18 compares the effect of the nucleation rate and threshold parameter. The green and magenta curves represent an order of magnitude difference in this input parameter. As expected, the higher F_N / N_I (green curve) leads to earlier failure because cavities form earlier and more rapidly. The increase in cavity density (bottom plot) is dramatic; cavities nucleate almost immediately and growth rapidly. Integration points begin to reach the maximum cavity number density (user input, $1,000N_I$ here) at 1,000 h for the $F_N / N_I = 2 \times 10^5$ simulation but not until right before failure around 4,000 h for the $F_N / N_I = 2 \times 10^4$ simulation. The effect of F_N / N_I on the cavity growth is much smaller (middle plot). The larger F_N / N_I nucleates cavities earlier, thus the initial increase in the maximum cavity size (in these simulations, cavities cannot grow until the nucleation threshold is met). The delayed onset of cavity growth with the smaller F_N / N_I is quickly overcome however and the two simulations have similar maximum cavity sizes for a few hundred hours. Thereafter, with the larger nucleation rate the porosity reaches a critical level (onset of coalescence) earlier, driving more rapid cavity growth. Note that an order of magnitude increase in F_N / N_I has a very similar effect on the cell strain rate as an order of magnitude increase in the diffusivity although F_N / N_I affects this change through the cavity spacing and the diffusivity through the cavity size.

2.3.6 Maximum cavity density

The maximum cavity density (N_{max}), as a multiple of the initial cavity density (N_I), may be user-limited or effectively bounded only by cavity coalescence. The maximum theoretical value of N_{max} / N_I is $(b_0 / a_0)^2$. This bound is based on (1) the maximum value of a / b is 1.0 and (2) the minimum value of a is a_0 . For $a_0 = 50$ nm and $b_0 = 60$ μ m, the theoretical bound for N_{max} / N_I is 1.4×10^6 ; i.e., the cavity density may increase by a factor of more than a million. Of course, this bound is neither physically realistic nor numerically attainable. The porosity limit of 1.0 is approached both as b decreases and a increases; thus the average cavity volume increase limits the number of cavities that may nucleate.

Figure 2-19 examines the effect of the N_{max} / N_I input parameter, over a range that varies from 10 to 1,000. The initial cavity density is 88 cavities/mm². With $N_{max} / N_I = 1,000$, the strain rate (upper left plot) reaches a minimum around 2,000 h and failure occurs at 10,000 h. Decreasing N_{max} / N_I to 100 does not have much effect on the time to minimum strain rate but the time to

failure triples to 30,000 h. With N_{max} / N_I set to 10, the minimum strain rate occurs around 50,000 h and failure has not yet occurred by the end of the simulation at 200,000 h.

The upper right figure tracks the evolution of the maximum computed cavity density. With the imposed limit of $N_{max} / N_I = 10$, one or more grain boundary integration points reach the maximum cavity density after only 20 hours; all further grain boundary opening occurs only through expansion of existing cavities. Indeed, even the average cavity density (not shown) becomes essentially constant after 2,000 hours. With N_{max} / N_I of 100, the limit is first reached at 2,000 hours, although the average density does not start to level off until 10,000 hours. Setting N_{max} / N_I to 1000 does not constrain nucleation for this set of material, loading, and geometric inputs. None of the integration points reach the imposed cavity density by the end of the simulation (cell failure). At least one integration point approaches the nucleation limit, with a maximum N / N_I greater than 800 but the average N / N_I at failure is only 100. A simulation with $N_{max} / N_I = 10^6$ confirms this effect; the higher nucleation limit yields identical results to the $N_{max} / N_I = 1,000$ case because the lower value does not limit nucleation. Thus the results with $N_{max} / N_I = 10^6$ are omitted from the plots for clarity.

The lower left figure demonstrates the effect of the cavity density limit on the cavity size. As expected, the curves are coincident until about 1,000 hours; cavity growth is unimpeded by the cavity density. After 1,000 hours, the cavity density for the $N_{max} / N_I = 1,000$ case first increases the cavity volumetric growth because the diffusion-based cavity growth rate increases as the porosity increases. However, the cavity density ultimately limits the cavity size as the porosity limit of 1.0 is reached. If N reaches N_{max} before coalescence the maximum value of a / a_0 is $1 / (\sqrt{N_{max} / N_I} \times a_0 / b_0)$. The $N_{max} / N_I = 10$ and 100 cases reach the respective a / a_0 limits of 120 and 380.

The sharp increases in cavity size (at 5,000, 20,000 and 100,000 hours for the three different cases) arise as the porosity reaches the level that triggers coalescence accelerated rapid cavity growth. The lower right figure presents the percentage of grain boundary elements with $a / b > 0.5$. The curves begin at the first time point for which at least one grain boundary element has $a / b > 0.5$. Note that these time points correlate with the nearly vertical segments of the $(a / a_0)_{max}$ curves in the lower left figure.

The values of N_{max} / N_I in the study explore the full range of the role of this parameter. The values correspond to maximum cavity densities from 880 to 88,000 cavities/mm² and minimum cavity spacing ($2b_{min}$) from 4 to 40 μm . The higher end of this range correlates well with recommendations based on literature study of experimental data on Grade 91 specimens, which indicates final cavity spacing of 30-70 μm , but acknowledges that reported values are average values and not necessarily from the failure surface which may indeed have smaller final cavity spacing before coalescence and failure.

2.3.7 Traction-influenced nucleation

The results and discussion above related to nucleation parameters focus on simulations for nucleation that depends on strain (and strain rate) but not directly on normal traction; *i.e.*, $\beta = 0$. As summarized in [12], while some experimental results support this $\beta = 0$ model, van der Giesen and colleagues, *e.g.*, [11] employ $\beta = 2$. When $\beta \neq 0$, the traction normalization parameter, Σ_0 affects the onset and rate of nucleation, in contrast to $\beta = 0$ parameter sets for which the value of Σ_0 is irrelevant.

Dodds *et al.*, [12] demonstrate that using $\beta = 2$ can focus nucleation and cavitation (and thus failure) to grain boundaries perpendicular (or nearly so) to the loading direction. The current work investigates the role of this parameter in differentiating the creep response for different applied stress levels. Chapter 6 provides much more detail on simulating a wide range of applied stresses but it is introduced here to demonstrate the role of these interface-cohesive material properties.

Figure 2-20 present cell strain histories at multiple applied stress levels (100-160 MPa) for both $\beta = 0$ and $\beta = 2$ cohesive model parameter sets. Note that these simulations use the crystal plasticity model for the grains rather than the Norton-Bailey model. Chapter 3 and 6 provide much more information about the crystal plasticity model, and its interaction with the grain boundary cohesive model. Here, let it simply serve as representative behavior in the current discussion of traction effects on nucleation. The cohesive model parameters are consistent between the two sets of results also, except for the nucleation traction exponent β .

The top plot shows the $\beta = 0$ simulation results along with experimental data at the same applied stress levels. The simulation results at the lower three stresses clearly reach tertiary creep and imminent failure. The 160 MPa case fails prematurely due to convergence difficulties with the CP model, but close examination of the results indicates that the strain rate has begun increasing. While the simulations reproduce the key features of the experimental data, there are discrepancies in the tertiary creep fit. With $\beta = 0$, the lower the applied stress the earlier the simulation predict cell failure with respect to the experimental data. Tweaking the parameters to better fit the low stress data has a detrimental effect on the higher stress simulations; the time-to-failure becomes longer than the measured result. Setting $\beta = 2$ (lower plot) improves the simulations ability to fit the experimental data over the range of applied stresses by providing more differentiation based on the magnitude of the grain boundary tractions. With $\beta = 2$, nucleation occurs earlier and faster for higher tractions than lower tractions, for the same strain and strain rate.

2.3.8 Summary

The grain boundary cohesive model provides the following functionality for simulating the phases of creep deformation.

- Early grain boundary viscous sliding leads to stress concentrations at triple points that enhance strain rates during the primary creep phase relative to simulations without grain boundary sliding or with free sliding. As continued sliding relaxes these stress concentrations, creep strain rates diminish and the cell settles into secondary creep.

- The nucleation threshold prevents appreciable cavity formation and growth until sufficient strain has accumulated on a grain boundary. This allows the secondary creep regime to be governed almost entirely by grain deformation.
- Grain boundary cavitation drives the tertiary creep phase and cell failure. The initially slow cavity nucleation and growth rapidly accelerates as cavities coalesce, eliminating the traction (both normal and tangential) carrying capacity of a grain boundary.

Some of the parameters are based on experimental measurements of the microstructure alone while other parameters depend on final or history dependent measurements. Diffusivity and the initial cavity spacing and size can potentially be measured from as-delivered specimens. The RVE response is independent of the precise value of the initial cavity size, at least within a reasonable range based on actual microstructural measurements. However, the time-to-failure is quite sensitive to both the diffusivity and initial cell spacing and the experimental data support sizable ranges in these parameter values.

The four nucleation parameters provide significantly flexibility to calibrate the interface-cohesive model. The nucleation threshold and rate parameter, F_N , the maximum cavity density N_{max} , and the traction-inclusion parameter β can strongly affect the minimum strain rate, the onset of tertiary creep and time-to-failure for a given set of microstructurally-based a_0 , b_0 , and D values. Estimates of N_{max} and β potentially can be obtained from post-failure microstructural measurements by examining the variation of cavity densities based on the grain boundary orientation with respect to the loading direction. This leaves F_N as the sole cavitation parameter without a history-independent microstructural basis (noting that F_N and Σ_0 are essentially a single parameter; appearing always as F_N / Σ_0^β). Experimental determination of F_N would require measurement of the onset of cavity nucleation or changes in cavity density under continued loading.

The cohesive interface model, with cavity nucleation and growth defining the normal traction-deformation response and linear viscous behavior for the tangential response, effectively represents the behavior of PAGBs in Grade 91 steels. Numerical accuracy and stability improvements in the cohesive model, and in the crystal plasticity model, allow these microstructure and mechanism-based responses to trace the creep response through all three phases up through microcrack formation. Future improvements would include end-of-life modeling changes (e.g., element extinction) and using additional alloy-specific test data to aid parameter calibration.

2.4 Chapter figures

Figure 2-2. 3D RVE model for simulating creep failure of Grade 91 steels.

Figure 2-3. Effect of grain boundary cohesive model linear stiffness on RVE strain rate noise and non-physical oscillations.

Figure 2-4. Grain boundary cohesive model normal traction (T_n) update procedure overview

Figure 2-5. Grain boundary cohesive model normal traction update procedure with (potentially) active cavitation

Figure 2-7. Effect of linear stiffness on traction oscillations and cell displacement. Contour plots show grain boundary normal traction values at end of 10 step loading ramp to 100 MPa uni-axial applied stress in 0.1 h for different interface normal stiffnesses. Line plot in lower right shows the displacement of the RVE surface ($Y = 0.2$ mm) during the load ramp. Grain boundary opening response is linear elastic (no cavitation) and tangential response is free sliding, $\eta_b = 10^2$ MPa $\cdot$ h $\cdot$ mm $^{-1}$.

Figure 2-8. Strain rate decomposition into grain boundary opening (green), grain boundary sliding (magenta), and grain deformation (blue) contributions for two linear stiffness values. RVE model with 140 MPa applied stress, linear-elastic grain normal opening response, $\eta_b = 10^6$ MPa $\cdot$ h $\cdot$ mm $^{-1}$.

Figure 2-9. Grain boundary normal opening model (a) linear-only response (no cavitation) compared to model with immediate transition from linear to cavitation-based response at nucleation and (b) opening model that maintains linear response but superposes the cavitation response after nucleation shown along with the responses shown in (a) above. RVE model with 140 MPa applied stress, $\eta_b = 10^6$ MPa $\cdot$ h $\cdot$ mm $^{-1}$, $K_{lin} = 10^7$ MPa/mm.

Figure 2-11. Effect of $q_{\min}$ on simulation failure time. Upper plot and inset show the cell strain rate, lower plot shows the cell strain. The three curves in each plot are coincident until the numerical simulations fail to converge.

Figure 2-12. Typical time to numerical failure with CP model for grains and cavitation model on grain boundaries. Circle markers are test data from Kimura [23]. Solid lines are numerical simulation results, While the simulations do not reach high strain rates at failure, the minimum strain rate and onset of tertiary creep are clear.

Figure 2-14. Normal tractions on elements with $a/b > 0.9$. Terminal step (3,300 h) of 140 MPa simulation with CP model and GB cavitation model with $\eta_b = 10^6 \text{ MPa} \cdot \text{h} \cdot \text{mm}^{-1}$, $K_{lin} = 10^7 \text{ MPa/mm}$.

Figure 2-15. RVE strain rate history for various grain boundary interface response general definitions. Applied uniaxial stress on $Y = 0.2$ mm surface ramped to 140 MPa in 0.1 h, then held for the remainder of the simulation. The grain response uses the the Norton-Bailey model with $B = 4 \times 10^{-18}$ MPa $^{-n} \cdot \text{h}^{-1}$ units and $n = 5$. The interface linear normal stiffness, K_{lin} is 10^7 MPa/mm. The cavitation and nucleation parameters are: $a_0 = 50$ nm, $b_0 = 60$ μm , $D = 10^{-15}$ MPa $^{-1} \cdot \text{h}^{-1} \cdot \text{mm}^3$, $\Sigma_0 = 200$ MPa, $F_N / N_I = 2 \times 10^4$, $N_{max} / N_I = 1,000$.

Figure 2-16. Effect of initial cavity radius (a_0) and spacing (b_0) on (a) cell strain rate, (b) average cavity size (among all grain boundary integration points) and (c) average cavity spacing (among all grain boundary integration points). 140 MPa applied stress.

Figure 2-17. Effect of η_b on cell strain rate decomposition for (a) no sliding ($\eta_b = 10^{12}$ MPa-h/mm), (b) free sliding ($\eta_b = 10^2$ MPa-h/mm) and (c) moderate sliding ($\eta_b = 10^6$ MPa-h/mm). All 3 simulations have linear grain boundaries with $K_{lin} = 10^7$ MPa/mm, Norton-Bailey grain creep response, 140 MPa applied stress.

Figure 2-18. Effect of diffusivity (D) and nucleation rate parameter (F_N / N_I) on (a) cell strain rate, (b) maximum cavity size (among all grain boundary integration points), relative to initial cavity size and (c) maximum number of cavities (among all grain boundary integration points), relative to initial number of cavities.

Figure 2-19. Effect of grain boundary nucleation parameter N_{max}/N_I input parameter on (a) cell strain rate, (b) maximum number of cavities (among all grain boundary integration points), relative to initial number of cavities, (c) maximum cavity size (among all grain boundary integration points), relative to initial cavity size, and (d) percentage of grain boundary elements with $a/b > 0.5$.

Figure 2-20. Effect of traction-influenced nucleation on stress-level differentiation of cell strain history. CP grain material response. Top plot results from $\beta = 0$ in nucleation model and bottom plot results from $\beta = 2$ in nucleation model. All other material parameters are the same for both plots. Each plot presents four simulation results (at 100, 120, 140, and 160 MPa applied uniaxial stress on $Y = 0.2$ mm cell surface) represented with solid lines and four sets of experimental results [23] (at same applied stresses) represented with circle markers and dashed lines.

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3 Modeling Grain Deformation using Crystal Plasticity

This section discusses the development of the crystal plasticity finite element modeling framework accounting for the effects of dislocation substructure evolution and the transition of dominant deformation mechanisms that are vital to characterizing the evolution of the creep resistance of Grade 91 during service life [24]. The use of crystal plasticity to model the inelastic response within the grains of the microstructure accounts for crystalline anisotropy, which gives rise to preferential directions of plastic strain. Also, capturing the correct stress-dependence for the creep strain within grains arising from competing mechanisms plays a key role in quantifying the local stress and strain states that promote the actual evolution of defects such as cavities along grain boundaries.

The following section describes the crystal plasticity framework for Grade 91 steel in relation to key microstructural features such as the crystallographic relationships of prior austenite grains. Section 3.2 follows with past developments of the crystal plasticity framework prior to this report. These developments include the enhancement of the CP numerical formulation and subsequent implementation in WARP3D, the inclusion of dislocation density-based constitutive equations with multiple hardening variables, initial studies of the strain-gradient enhanced formulations to model Bauschinger effects produced by geometrically necessary dislocations, statistically stored dislocation density-based modeling of Grade 91, and derivation of effective power-law exponent for grain boundary model nonlocal effects. Then, Section 3.3 describes the additional enhanced features of the CP finite element framework in WARP3D, the multi-mechanism constitutive relations for modeling plasticity and creep within PAG of Grade 91, and the estimation of material parameters within those relations by fitting steady-state strain rate curves at different stresses to experimental creep tests. These constitutive relations and material parameters are employed to predict the creep response of the material for fully-resolved microstructural models similar to those reported in Chapter 6. Lastly, conclusions of the crystal plasticity modeling effort and possible extensions of the framework are discussed in Section 3.5.

3.1 Overview of crystal plasticity modeling framework in relation to microstructural features

As described in Chapter 1 the microstructure of Grade 91 consists of a complex hierarchy of defect structures with increasingly finer spatial dimensions. During the normalizing process, the prior austenite grains (PAG) transform to lath martensite, and fractions of each grain interior experience different lattice transformations that are approximated by the Kurdjumov-Sachs misorientation relationship [25]. These regions of distinct martensite variants are referred to as packets, which have similar lath morphology but possibly high angle lattice mis-orientation. A substantial amount of dislocation density is also generated during the normalizing process and self organizes into structures, the largest of which are called blocks. Within blocks, alternating patterns of densely packed and immobilized dislocations interspaced by relatively uninterrupted atomic lattice are observed and are termed as laths [24]. Due to their geometrical arrangement, the laths are often called dislocation cells, and the regions of high and low dislocation densities are termed cell

walls and cell interiors, respectively. This hierarchical network of dislocations, packet boundaries, and PAG boundaries provides substantial barriers to motion of mobile dislocation density and thus high resistance to creep. Recovery of this network occurs at high temperatures and sustained mechanical stress, leading ultimately to creep rupture. Therefore, to develop capabilities for predicting the useful service life of Grade 91, a crystal plasticity finite element modeling framework is developed to capture the recovery processes of these microstructural features.

This report describes models for microstructural evolution consisting of representative volume elements (RVE) containing many finite elements arranged in patterns to approximate the PAG. Similar microstructural models using both 2D (plane-strain) and 3D realizations were developed previously [12] with emphasis on the grain boundary deformation mechanisms. Due to the prohibitive expense of resolving length scales across several orders of magnitude, only the PAG will be explicitly represented. An example microstructure containing 100 grains each composed of several finite elements is described in Section 3.2.6. The lattice orientations of all finite elements within a single grain are assigned a common value at the start of numerical simulations. The crystal lattice of the martensite phase is a body-centered tetragonal (BCT) crystal, which will be approximated herein as a body-centered cubic (BCC) structure. The most commonly active slip systems for BCC crystals are the 12 $\{1\bar{1}0\}\langle 111 \rangle$ systems, 12 $\{11\bar{2}\}\langle 111 \rangle$ systems, and 24 $\{12\bar{3}\}\langle 111 \rangle$ systems, for a total of 48 systems. The motion of dislocations in directions specified by these slip systems leads to anisotropic response that is expected to affect the stress distribution within grains and along boundaries in contrast to the isotropic Norton-Bailey model employed in Chapter 2.

In the crystal plasticity finite element method, the plastic slip of dislocations is driven by the resolved shear stress $\tau^{(s)}$ on each slip system (s), as described in 3.2.2. This motion gives rise to the observed creeping deformation of the material during experiments. Dislocation slip is impeded by several barriers within the blocks and laths which must be accounted for in the constitutive model. The primary mechanism of dislocation motion at moderate stress and high temperature is the alternating glide and climb of dislocations around pinning obstacles [26]. Climb and glide permit mobile dislocation motion toward sites both within and at the boundaries of subgrain structures, where dipole-coalescence-based dislocation recovery mechanisms take place. The scale of low-angle subgrain structures also coarsens as the dislocations comprising their boundaries are mobilized by climb and glide, often doubling from initial as-tempered dimensions. The extent of microstructural recovery grows with the scale of inelastic strain that is accommodated by dislocation climb and glide. Efforts were undertaken during this project to account for these interacting mechanisms of dislocation mobility and substructure evolution within the crystal plasticity constitutive model for the PAG. One stage of the constitutive modeling framework, described in Section 3.2.4, is based on tracking the evolution of the total dislocation density as partitioned to the individual slip systems within the body centered cubic (BCC) lattice. This model features several mechanisms for dislocation evolution, such as thermally-activated recovery by dislocation climb and dipole capture, and it also captures the crystallographic distribution of the

dislocation network with high fidelity. However, during preliminary studies, this computational model did not reproduce the stress-dependence of the minimum creep strain rate reported from creep tests of Grade 91, and the evolution of strain rate within the grains varied only by one magnitude compared to the several magnitudes exhibited by the experimental datasets.

Therefore, a revised crystal plasticity for climb and glide is developed in Section 3.3.2 using a power-law flow rule with a hardening term reflecting the immobilization of mobile dislocation density that is initially present after processing of Grade 91. Additionally, experimentally obtained creep strain rates at lower stresses [27] suggest a deformation mechanism transition occurs below 100 MPa stress at 600 C temperature. These trends motivated the incorporation of terms reflecting diffusional flow within the grains. With any diffusional mechanism, the key idea is that there is a lattice flux of mass (atoms going one way, or, equivalently, vacancies going the other), with “sources” and “sinks” marking the beginnings and endings of the respective lattice journeys. The difference in chemical potential between the endpoints provides the driving force; usually the endpoints are taken to lie on internal (or external) interfaces such as grain boundaries, and a major part of the driving force is the normal stress on the boundary. While the local effects of atomic diffusion are not followed in detail by the continuum treatment of viscoplasticity, a first order approximation is achieved by using a linear viscous deviator stress within the grains to provide a second source of inelastic strain rate. This multi-mechanism model for the creep deformation of Grade 91 developed in Section 3.3.2 is investigated through a series of virtual creep tests both in 3.4 and Chapter 0. This CP modeling framework provides enhanced capabilities compared to the isotropic Norton-Bailey model for resolving the distribution of stress within the prior austenite grains and other substructure features. Predicting the evolution of these driving stresses is crucial for capturing both the loss of creep resistance within the grains as well as the local stress state along grain boundaries that influences the rates of cavity nucleation and growth.

3.2 Summary of prior developments for crystal plasticity model of grain response

In pursuit of the grain deformation modeling framework described in Section 3.1, a comprehensive dislocation density-based crystal plasticity computational framework has been developed in previous project years to capture the deformation mechanisms of Grade 91 during creep behavior. These efforts, including extensions to model geometrically necessary dislocation effects, are recorded in a previous report [12] and are summarized here to provide background for the combined dislocation creep and diffusion model in Section 3.3.2.

Sections 3.2.1 and 3.2.3: A common platform for crystal plasticity model testing was developed both in WARP3D and a pre-existing MATLAB finite element code. Also, the computational aspects of geometric necessary dislocation (GND) density modeling in the crystal plastic finite element method were studied using a new formulation employing Lie-algebra mappings and nodal projection of elastic rotation.

Sections 3.2.2 and 3.2.3: Significant enhancements were performed for the crystal plasticity material model platform in WARP3D to accommodate multi-variable hardening models by generalizing the framework of the constitutive equations and also the relevant subroutines in the code. Additionally, the robustness of the material subroutine was improved by adding state predictors as well as finite difference tangent check routines. The new constitutive framework was verified for a reference model for aluminum proposed by Ma et al. [28], which has a mechanism-based treatment of the dislocation density evolution.

Sections 3.2.2, 3.2.5, and 3.2.6: A dislocation density-based crystal plasticity model was developed for Grade 91 by retaining some features of the previous model [28] but substituting the hardening mechanism for a term based on dislocation climb-glide over precipitates and adding the body-centered cubic slip systems. Other algorithmic enhancements were performed, such as including an extended nonlinear equation solver package [29] and systematic bookkeeping of history variables.

3.2.1 Translation of material subroutine from WARP3D to MATLAB

To facilitate the investigation of the crystal plasticity modeling framework, the entire material subroutine from WARP3D was translated and implemented into a previously-developed research finite element code written in MATLAB, which provides debugging features and simplified syntax compared to FORTRAN. This code is capable of performing fully nonlinear finite element analyses for small and medium size problems and is fully customizable in terms of element subroutines, internal/history variable storage, and external macros. At the time of translation, only the Mechanical Threshold Strength (MTS) model [14] [30] was implemented in WARP3D. First, the MTS crystal plasticity model had to be ported from WARP3D into MATLAB, which was performed line-by-line in converting syntax from .f files to .m files. The new material subroutine was subsequently verified by comparing the output for several test problems between WARP3D and MATLAB codes. The MATLAB code streamlined the later prototyping of constitutive models, such as the diffusional creep model in Section 3.3.2.

3.2.2 Kinematic description and multi-variable hardening model framework in WARP3D

The crystal plasticity model platform in WARP3D has been extended to the multi-variable case by generalizing the constitutive equations and relevant subroutines in the code. These features are important for modeling the creep response of Grade 91 by allowing variable evolution of dislocation densities on different slip systems. Additionally, enhancements were added to the nonlinear equation solver in the material subroutine to improve its robustness and also to streamline the implementation of constitutive models.

A brief discussion of the relevant kinematic assumptions for the implementation of crystal plasticity in the finite element program WARP3D [14] is given below. Further details are contained in [12] and [30]. The treatment of large-strain constitutive modeling takes the form of hypoelasticity (also called the rate form) based upon an objective update of the Cauchy stress tensor

σ on the current deformed state. The particular objective stress rate employed by WARP3D is the Green-Naghdi rate, $\dot{\sigma}$, expressed in terms of the spin tensor Ω as follows:

$$\dot{\sigma} = \dot{\sigma} + \sigma\Omega - \Omega\sigma \quad (3.1)$$

where σ is the Cauchy stress tensor, the superimposed “dot” denotes the material time derivative, and the spin tensor $\Omega = \dot{R}R^T$ is defined in terms of the rotation tensor R from the polar decomposition of the deformation gradient $F = RU$.

Within crystal plasticity theory, the plastic deformations are characterized by motion of dislocations within the crystal lattice. This mode of deformation is traditionally described in continuum mechanics through the multiplicative split of the deformation gradient into elastic and plastic parts:

$$F = F^e F^p \approx (I + \varepsilon) R^e R^p U^p \quad (3.2)$$

where the additional assumption of small elastic strains $\varepsilon \ll I$ is employed to simplify the resultant formulation. This assumption is realistic for the behavior of metals in the creep regime.

Substituting the elasto-plastic kinematic representation (3.2) into the Green-Naghdi objective rate and transforming to the unrotated intermediate configuration leads to the following rate equation:

$$\dot{t} = C_o : (d - \bar{d}^p) + R\bar{w}^p R^T t - t R\bar{w}^p R^T \quad (3.3)$$

in which $t = R^T \sigma R$ is the unrotated Cauchy stress and $d = \frac{1}{2}(\dot{U}U^{-1} + U^{-1}\dot{U})$ is the unrotated rate of deformation.

For single crystal plasticity, the plastic strain rate is commonly represented through slip rates $\dot{\gamma}^{(s)}$ resolved onto the primary crystallographic planes $s = 1, \dots, n_{slip}$:

$$\tilde{t}^p = \sum_{s=1}^{n_{slip}} \dot{\gamma}^{(s)} (\tilde{b}^{(s)} \otimes \tilde{n}^{(s)}) \quad (3.4)$$

$$\bar{d}^p = \sum_{s=1}^{n_{slip}} \dot{\gamma}^{(s)} R^{pT} \tilde{m}^{(s)} R^p \quad (3.5)$$

$$\bar{w}^p = \sum_{s=1}^{n_{slip}} \dot{\gamma}^{(s)} R^{pT} \tilde{q}^{(s)} R^p \quad (3.6)$$

$$\tilde{\mathbf{m}}^{(s)} = \text{sym}(\tilde{\mathbf{b}}^{(s)} \otimes \tilde{\mathbf{n}}^{(s)}) \quad (3.7)$$

$$\tilde{\mathbf{q}}^{(s)} = \text{skew}(\tilde{\mathbf{b}}^{(s)} \otimes \tilde{\mathbf{n}}^{(s)}) \quad (3.8)$$

where $\tilde{\mathbf{b}}^{(s)}$ is the slip direction within a crystal plane s and $\tilde{\mathbf{n}}^{(s)}$ is the unit normal to plane s . The “tilde” overbar refers to quantities in the lattice frame while the flat overbar denotes quantities in the current deformed frame. Additionally, the evolution of the plastic rotation rate is expressed through the plastic vorticity as $\dot{\mathbf{R}}^p = \bar{\mathbf{w}}^p \mathbf{R}^p$.

Many different constitutive expressions have been proposed for relating the plastic slip rates $\dot{\gamma}^{(s)}$ to the current applied stress $\boldsymbol{\sigma}$ and other factors such as temperature and microstructural state. To allow for further model development, a general form of the slip rates is considered:

$$\dot{\gamma}^{(s)} = \dot{\gamma}^{(s)}(\tau^{(s)}, \xi, \mathbf{d}; \mathbf{v}) \quad (3.9)$$

where

$$\tau^{(s)} = \mathbf{t} : (\mathbf{R}^{pT} \tilde{\mathbf{m}}^{(s)} \mathbf{R}^p) \quad (3.10)$$

is the resolved shear stress on the slip system, ξ is a set of hardening variables, and $\mathbf{d}$ is the unrotated rate of deformation defined previously. These three fields will be treated in an implicit fashion within the computational algorithm, meaning that a coupled system of nonlinear equations will be solved at each time step. Additionally, the model can accommodate other parameters and field dependencies that are treated in an explicit manner; these variables are denoted by $\mathbf{v}$. An example of this field is the Nye tensor $\boldsymbol{\alpha}$ discussed within Section 3.2.3 and [12] concerning the size-dependent features of the MTS constitutive model.

The second major component of the model is the evolution of the hardening variables ξ , which is considered in a format similar to (3.9):

$$\dot{\xi} = \dot{\xi}(\mathbf{t}, \xi, \mathbf{d}; \mathbf{v}) \quad (3.11)$$

In the finite element setting, the material evolution equations (3.3) and (3.11) are tracked at the integration points of the elements within the mesh at a series of time steps. Therefore, the objective of the material update routine is to advance the values of the stress and hardening variables at time t_n to time $t_{n+1} = t_n + \Delta t$. Both equations (3.3) and (3.11) will be integrated using a backward Euler scheme, and together represent an implicit system of equations to be solved. The equations are:

$$\mathbf{0} = \mathbf{R}_1 = \mathbf{t}_{n+1} - \bar{\mathbf{t}}(\mathbf{t}_{n+1}, \xi_{n+1}, \Delta \mathbf{d}_{n+1}; \mathbf{v}_n) = \mathbf{t}_{n+1} - \left[\mathbf{t}_n + \dot{\mathbf{t}}(\mathbf{t}_{n+1}, \xi_{n+1}, \Delta \mathbf{d}_{n+1}; \mathbf{v}_n) \Delta t \right] \quad (3.12)$$

$$\mathbf{0} = \mathbf{R}_2 = \xi_{n+1} - \bar{\xi}(\mathbf{t}_{n+1}, \xi_{n+1}, \Delta \mathbf{d}_{n+1}; \mathbf{v}_n) = \xi_{n+1} - \left[\xi_n + \dot{\xi}(\mathbf{t}_{n+1}, \xi_{n+1}, \Delta \mathbf{d}_{n+1}; \mathbf{v}_n) \Delta t \right] \quad (3.13)$$

where $\Delta \mathbf{d}_{n+1} = \mathbf{d}_{n+1} \Delta t$ is specified from the current best estimate of the nodal displacement increment. Note the explicit internal variables $\mathbf{v}$ do not require a system of equations because these values are supplied or computed offline from the material update algorithm.

The quantities within the objective stress update (3.12) are defined with respect to the time discrete counterparts of (3.3) – (3.10):

$$\dot{\mathbf{t}}_{n+1} \Delta t = \mathbf{C}_o : (\Delta \mathbf{d}_{n+1} - \Delta \bar{\mathbf{d}}_{n+1}^p) + \Delta \bar{\mathbf{W}}_{n+1}^p \mathbf{t}_{n+1} - \mathbf{t}_{n+1} \Delta \bar{\mathbf{W}}_{n+1}^p \quad (3.14)$$

$$\Delta \bar{\mathbf{d}}_{n+1}^p = \sum_{s=1}^{n_{slp}} \Delta \gamma_{n+1}^{(s)} \mathbf{R}_n^{pT} \tilde{\mathbf{m}}^{(s)} \mathbf{R}_n^p \quad (3.15)$$

$$\Delta \bar{\mathbf{W}}_{n+1}^p = \mathbf{R}_{n+1} \left[\sum_{s=1}^{n_{slp}} \Delta \gamma_{n+1}^{(s)} \mathbf{R}_n^{pT} \tilde{\mathbf{q}}^{(s)} \mathbf{R}_n^p \right] \mathbf{R}_{n+1}^T \quad (3.16)$$

$$\Delta \gamma_{n+1}^{(s)} = \dot{\gamma}^{(s)}(\tau_{n+1}^{(s)}, \xi_{n+1}, \Delta \mathbf{d}_{n+1} / \Delta t; \mathbf{v}_n) \Delta t \quad (3.17)$$

$$\tau_{n+1}^{(s)} = \mathbf{t}_{n+1} : (\mathbf{R}_n^{pT} \tilde{\mathbf{m}}^{(s)} \mathbf{R}_n^p) \quad (3.18)$$

Notice that the plastic rotation tensor $\mathbf{R}^p$ is also treated in an explicit fashion since the value from time t_n is used in equations (3.15) – (3.18). This algorithmic assumption greatly simplifies the nonlinear system of equations (3.12) – (3.13) and generally appropriate since the evolution of plastic rotations $\mathbf{R}^p$ is relatively slow compared to the plastic strain rate $\bar{\mathbf{d}}^p$ [30].

The residual equations (3.12) – (3.13) are solved using a Newton-Raphson scheme with appropriate initial guesses for the stress $\mathbf{t}_{n+1}$ and hardening ξ_{n+1} . Details of the algorithm are provided in [12]. The Jacobian matrix, which has dimensions $6 + n_{hard} \times 6 + n_{hard}$, is obtained from the consistent linearization of (3.12) – (3.13), where special care is taken to apply the chain rule of calculus to isolate the single terms which are dependent on the specific form of the constitutive model. Clearly, only six quantities are required to be implemented by the user:

$$\Delta\gamma_{n+1}^{(s)}, \dot{\xi}_{\beta=1, n_{hard}}, \frac{\partial \Delta\gamma_{n+1}^{(s)}}{\partial \tau^{(s)}}, \frac{\partial \Delta\gamma_{n+1}^{(s)}}{\partial \xi_{\beta}}, \frac{\partial \dot{\xi}_{\alpha}}{\partial t_{kl}}, \frac{\partial \dot{\xi}_{\alpha}}{\partial \xi_{\beta}} \quad (3.19)$$

These six quantities are the slip increment (3.9), hardening evolution rate (3.11), and the partial derivatives of these two fields with respect to the primary unknowns $\mathbf{t}$ and ξ . Each of these depends integrally upon the specific form of the constitutive model.

When the Newton-Raphson algorithm has been terminated after sufficient reduction of the residuals, the consistent values for $\mathbf{t}$ and ξ have been found for the current value of the strain increment $\Delta\mathbf{d}_{n+1}$ at the integration point. The unrotated stress $\mathbf{t}$ is then transformed to the Cauchy stress σ and used by the element subroutine to compute the internal force vector for assembly in the global equilibrium residual vector.

Often, the evolution equations (3.12) – (3.13) represent a very stiff system of equations [31], particularly when the plastic slip rate (3.9) as a function of the resolved shear stress is expressed as an exponential form rather than power-law form. Therefore, several enhancements have been added to the finite element solution algorithm in WARP3D that facilitate the solution of stiff systems [12]. The current global finite element solver in WARP3D employs a Newton-Raphson approach with adaptive subdivision of the time step Δt if a Gauss point of an element fails to converge within the material stress update algorithm. Within the material stress update algorithm for crystal plasticity, the strain increment can also be adaptively subdivided to determine the converged stresses and hardening with intermediate increments. Also, the material update equations are in fact solved using the modified Newton method combined with line search. Lastly, the algorithmic material update is performed in two phases as described in [12]. First, an initialization phase is employed wherein the hardening variables are kept frozen at a best-estimate value while the stress is updated via (3.12). After convergence, the estimated stress and hardening are used as the initial guess for solving (3.12) – (3.13) at the current (sub)increment.

3.2.3 Modeling geometrically necessary dislocations through plastic rotation gradient field 90%

Grade 91 steel is known to exhibit cyclic softening during fatigue tests [32] [33] [34], where the maximum flow stress decreases and the total deformation increases over several hundred cycles. A viable approach for capturing these microstructural effects is through the geometrically necessary dislocation (GND) density based model proposed by Bayley and Geers [35], where the back stress is derived from the GND spatial gradient as:

$$\tau_b^{(\alpha)} = \tilde{\mathbf{b}}^{(s)} \cdot \left(\sigma_s^{\text{int}} + \sigma_e^{\text{int}} \right) \cdot \tilde{\mathbf{n}}^{(s)} \quad (3.20)$$

This model is based on the mechanism of dislocation pile up against grain boundaries. When the dislocation density varies spatially, the elastic field produced by individual dislocation can be

integrated within a small zone of influence to yield a resultant back stress. The derivations within [35] provide expressions for the back stress, which are highly dependent on the crystallographic orientation.

In order to calculate the GND density gradient, Bayley et al. employed a mixed formulation with dislocation density as nodal unknowns. However, that method is computationally expensive because each node in the mesh has 18 additional degrees of freedom (DOF) which must be included in the global system of equations. Currently, the architecture of WARP3D does not permit the addition of DOFs per node. Therefore, a simplified approximation is pursued in this work that is based only on displacement nodal unknowns and using projections of the elastic deformation gradient tensor to obtain the GND.

The measure of geometrically necessary dislocation density is obtained from the elastic incompatibility quantified by the Nye tensor α . The mapping of Nye tensor components into dislocation densities on slip systems is accomplished through a L^2 minimization process advocated by Arsenlis and Parks [36], leading to the following equation:

$$\rho_{GND} = (\mathbf{A}^T \mathbf{A})^{-1} \mathbf{A}^T \alpha = \mathbf{B} \alpha, \quad A_{ij}^{(s)} = \tilde{\mathbf{b}}_i^{(s)} \otimes \tilde{\mathbf{t}}_j^{(s)} \quad (3.21)$$

The Nye tensor is obtained from the gradient of the elastic deformation gradient $\mathbf{F}_e$:

$$\alpha = -\nabla_0 \times \mathbf{F}_e^{-1} \quad (3.22)$$

However, in the traditional finite element implementation of crystal plasticity, the elastic deformation gradient is treated as a local quantity that is calculated solely at the integration points inside elements of the mesh. Therefore, two techniques for projecting the elastic rotation tensor and evaluating its derivative were developed and compared through a series of benchmarks [37]. As a candidate crystal plasticity model, the Mechanical Threshold Strength (MTS) model that is implemented in WARP3D was chosen. The current implementation of the model [14] [30] uses an elemental projection to evaluate the derivatives for the Nye tensor.

Due to the assumption of small elastic strains (see (3.2)), the quantity which we need to interpolate in order to compute the Nye tensor $\alpha = \nabla \times \mathbf{F}^{e-1}$ is the elastic rotation tensor $\mathbf{R}^e$:

$$\mathbf{R}^e = \mathbf{R} [\mathbf{R}^p]^{-1}, \quad \mathbf{R} = \mathbf{F} \mathbf{U}^{-1} \quad (3.23)$$

where $\mathbf{R}^p$ is the plastic rotation tensor evaluated through the constitutive model and $\mathbf{R}$ is the rotation tensor defined from the right polar decomposition of the deformation gradient $\mathbf{F}$. For the elemental projection, the values of $\mathbf{R}^e$ at the Gauss points in each element are employed to fit a linear function for each component, and this linear function is differentiated to obtain the curl

$\nabla \times \mathbf{F}^{e-1}$. While the elemental projection was sufficient for conducting the simulations in Messner et al. [30], it is an ad hoc procedure. First, this element-based approach does not incorporate any communication of the field response between elements of the mesh, dampening the nonlocal contribution from the GND hardening term. Also, it is valid only for obtaining the first derivatives of the rotation tensor field. In contrast, crystal plasticity models involving a measure of the back-stress require the second derivative of the elastic rotation to be well-defined [38] [39].

In light of these motivations, a new numerical method is developed for extending the values of the plastic deformation gradient at the integration points into a non-locally defined field. The procedure is motivated by the developments of Mota et al. [40] on the projection of internal variables. First, the value of the plastic deformation gradient is obtained at each integration point by the usual loop over all the finite elements in the mesh during the stress-update process. These values are extrapolated to the nodes of the mesh by using the bilinear finite element shape functions, in a process directly analogous to the post-processing of elemental stress fields for contour plots. The multiple values of the field at each node, which are generated by the various elements neighboring that node, are then averaged to a single value based on the tributary area of the adjoining elements. This unique nodal value then forms a field that can be interpolated using the Lagrangian finite element shape functions. The derivative of the field is then obtained by directly differentiating the Lagrangian shape functions, specifically at the integration points of the finite element mesh. This provides the value of the oriented GND density that are needed within the evaluation of the material model listed above.

Although the node-based smoothing approach is conceptually straight-forward, an issue arises when the method is applied in its current form to the elastic rotation tensor. Recall that rotation tensors are a member of the space of orthonormal tensors $SO(3)$. This space of tensors is closed under multiplication (Lie group) rather than addition (Lie algebra), which means that linear interpolation produces tensors outside the space. A novel method for preserving the properties of internal variable fields is proposed in Mota et al. [40] which uses the associated Lie algebra space of skew tensors $so(3)$. Accounting for this mapping between Lie algebras and groups during the derivative evaluation, the modified procedure for computing the Nye tensor field $\boldsymbol{\alpha}$ is summarized in Table 3-1.

Table 3-1. Node-based procedure for computing Nye tensor

1. Logarithmic map:	$\mathbf{r}_a^e = \ln(\mathbf{R}_a^e)$ for each $a = 1, \dots, n_{\text{int}}$ in Ω_e
2. Elemental field:	$\hat{\mathbf{r}}^e(\boldsymbol{\xi}) = \sum_{a=1}^{n_{\text{int}}} \hat{\mathbf{r}}_a^e \hat{N}_a(\boldsymbol{\xi})$ in Ω_e
3. Extrapolate:	$\hat{\mathbf{r}}_{A,e}^e = \hat{\mathbf{r}}_a^e(\boldsymbol{\xi}_{A,e})$ for each $A = 1, \dots, n_{\text{node}}$ and Ω_e
4. Smooth:	$\tilde{\mathbf{r}}_A = \left(\sum_{e=1}^{n_{\text{el}}} \hat{\mathbf{r}}_{A,e}^e \right) / n_{\text{el}}^A$ for each $A = 1, \dots, n_{\text{node}}$
5. Interpolate:	$\tilde{\mathbf{r}}^e(\mathbf{X}_a) = \sum_{A=1}^{n_{\text{node}}} \tilde{\mathbf{r}}_A N_A(\mathbf{X}_a)$ for each $a = 1, \dots, n_{\text{int}}$ in Ω_e
6. Exponential map:	$\tilde{\mathbf{R}}^e(\mathbf{X}_a) = \exp(\tilde{\mathbf{r}}^e(\mathbf{X}_a))$
7. Differentiate:	$\nabla(\tilde{\mathbf{R}}^e)^T = \nabla[\exp(\tilde{\mathbf{r}}^e(\mathbf{X}_a))]^T$

An important feature affecting the accuracy, robustness, and stability properties of a constitutive material model is the explicit or implicit treatment of the material and kinematic quantities. The current implementation in WARP3D uses an implicit treatment of the stress tensor and hardening variables, but an explicit treatment of the kinematic variables $\mathbf{R}^e$ and $\boldsymbol{\alpha}$. As discussed in the WARP3D manual [14], the evolution of the elastic rotation tensor and Nye tensor are expected to be rather mild from one load step to the next in a typical crystal plasticity simulation. The benefit of performing explicit calculation is that an additional system of equations does not have to be solved self-consistently. However, the assumption of slowly varying rotations places a restriction on the size of the loading increment which may not always be so easy to determine a priori. Addressing this issue by reducing the load step size causes an increase in the number of stiffness matrix factorizations and greatly increases the cost of simulating the response.

As an alternative, a staggered procedure was developed for simultaneously solving for the stress tensor, hardening variables, and kinematic variables [37]. Observe that the calculation of the Nye tensor $\boldsymbol{\alpha}_n = \nabla \times \mathbf{R}_n^{e-1}$ necessarily involves nonlocal calculations, either across Gauss points or across nodes and elements. Therefore, this calculation must occur outside of the traditional loop over Gauss points for the material update. Rather than adding additional equations at the global Newton level, an internal loop is performed within each Newton iteration, referred to as the subcycle loop. A comparison of the performance properties and the level of solution equivalence between the elemental and nodal projection methods was assessed through a simulation of a single crystal loaded by shearing tractions. The size effect properties of the MTS model were investigated through the bending of a single crystal strip subjected to monotonically increasing rotations is investigated. The robustness of the method under heterogeneous deformations

indicate that it is a solid platform for modeling back stress effects from geometrically necessary dislocations.

3.2.4 Statistically-stored dislocation density based model including climb-glide mechanism

A dislocation density-based model was developed and implemented within the multi-variable crystal plasticity framework of WARP3D to capture the material response across a range of deformation modes including strain-driven tensile tests, creep-fatigue, and creep [12]. The constitutive model retains the dislocation geometrical interactions proposed in the Ma and Roters [28] model but accounts for other microstructurally relevant mechanisms for Grade 91 as described in Section 3.1. The slip systems for face-centered cubic (FCC) aluminum were replaced with the body-centered cubic (BCC) systems for martensitic steel. While dislocations in BCC crystals slip along the $[111]$ direction, the relative slip resistance offered along the (110) , (112) , and (123) planes are nearly equal, particularly at high temperatures [41]. Therefore, all 48 of these slip systems are utilized in the model; each system is listed in Table 3-2. The interaction of dislocations across slip systems is calculated geometrically through sine and cosine functions of the slip planes, defining parallel and forest dislocation contributions. Only statistically stored edge dislocations were considered in the crystal plasticity model.

Table 3-2. Slip system Miller indices for slip plane and direction for BCC crystals

ID	Slip System	ID	Slip System	ID	Slip System
(1)	$(110)[\bar{1}11]$	(2)	$(110)[1\bar{1}1]$	(3)	$(1\bar{1}0)[111]$
(4)	$(1\bar{1}0)[11\bar{1}]$	(5)	$(101)[11\bar{1}]$	(6)	$(101)[\bar{1}11]$
(7)	$(10\bar{1})[111]$	(8)	$(10\bar{1})[1\bar{1}1]$	(9)	$(011)[11\bar{1}]$
(10)	$(011)[1\bar{1}1]$	(11)	$(01\bar{1})[111]$	(12)	$(01\bar{1})[\bar{1}11]$
(13)	$(112)[11\bar{1}]$	(14)	$(\bar{1}12)[1\bar{1}1]$	(15)	$(1\bar{1}2)[\bar{1}11]$
(16)	$(11\bar{2})[111]$	(17)	$(121)[1\bar{1}1]$	(18)	$(\bar{1}21)[11\bar{1}]$
(19)	$(1\bar{2}1)[111]$	(20)	$(12\bar{1})[\bar{1}11]$	(21)	$(211)[\bar{1}11]$
(22)	$(\bar{2}11)[111]$	(23)	$(2\bar{1}1)[11\bar{1}]$	(24)	$(21\bar{1})[1\bar{1}1]$
(25)	$(123)[11\bar{1}]$	(26)	$(123)[1\bar{1}1]$	(27)	$(1\bar{2}3)[\bar{1}11]$
(28)	$(12\bar{3})[111]$	(29)	$(132)[1\bar{1}1]$	(30)	$(\bar{1}32)[11\bar{1}]$
(31)	$(1\bar{3}2)[111]$	(32)	$(13\bar{2})[\bar{1}11]$	(33)	$(213)[11\bar{1}]$
(34)	$(\bar{2}13)[1\bar{1}1]$	(35)	$(2\bar{1}3)[\bar{1}11]$	(36)	$(21\bar{3})[111]$
(37)	$(231)[1\bar{1}1]$	(38)	$(\bar{2}31)[11\bar{1}]$	(39)	$(2\bar{3}1)[111]$
(40)	$(23\bar{1})[\bar{1}11]$	(41)	$(312)[\bar{1}11]$	(42)	$(\bar{3}12)[111]$
(43)	$(3\bar{1}2)[11\bar{1}]$	(44)	$(31\bar{2})[1\bar{1}1]$	(45)	$(321)[\bar{1}11]$
(46)	$(\bar{3}21)[111]$	(47)	$(3\bar{2}1)[11\bar{1}]$	(48)	$(32\bar{1})[1\bar{1}1]$

The relevant equations for the crystal plasticity model proposed for Grade 91 are listed in Table 3-3; details on the variable definitions and units are given in [12]. The flow rule has been modified from [28] to capture two key features of the material mechanisms. First, constitutive models for BCC materials [42] typically consider the lattice resistance or Peierls stress to be the most significant short-range obstacle to dislocation motion, which is taken as a constant stress $\hat{\tau}_0$ that does not depend on the dislocation network. Also, during creep at high temperatures under sustained lower stresses, the motion of dislocations may be described through a glide-climb mechanism [32] [43]. In this mechanism, the dislocations are pinned against precipitates or dense cell walls in the microstructure for extended periods. A distinguishing feature of the proposed model is that the mean free path actually evolves in time due to the coarsening of the $M_{23}C_6$ carbides and the spreading out of the subgrain cell walls. The coarsening rate for particles is modeled through the Ostwald ripening equation [44], which accounts for agglomeration together over time due to diffusion at high temperatures. However, the simulation results in [12] adopt a constant mean free path to focus the contribution to the creep rate acceleration to be the grain boundary cavitation alone.

Table 3-3. Flow rule and dislocation density evolution for Grade 91 constitutive model

Equation	Eqn. Number
$\dot{\gamma}^{(\alpha)} = \left(f_M \rho_{SSD}^{(\alpha)} \right) v_s \lambda^{(\alpha)} \times \exp \left[\frac{-F_o}{kT} \left(1 - \left\langle \frac{ \tau^{(\alpha)} - \tau_{pass}^{(\alpha)}}{\hat{\tau}_0 G/G_0} \right\rangle^p \right)^q \right] \text{sign}(\tau^{(\alpha)})$	(3.24) – Slip rate
$\lambda^{(\alpha)} = c_\lambda b \eta_{part}(t, T)$	(3.25) – Mean free path
$\tau_{pass}^{(\alpha)} = c_\rho G b \sqrt{\rho_p^{(\alpha)}}$	(3.26) – Passing stress
$\rho_F^{(\alpha)} = \sum_{\beta=1}^N \rho_{SSD}^{(\beta)} \left \cos(\tilde{\mathbf{m}}^{(\alpha)}, \tilde{\mathbf{t}}^{(\beta)}) \right $	(3.27) – Forest dislocations
$\rho_p^{(\alpha)} = \sum_{\beta=1}^N \rho_{SSD}^{(\beta)} \left \sin(\tilde{\mathbf{m}}^{(\alpha)}, \tilde{\mathbf{t}}^{(\beta)}) \right $	(3.28) – Parallel dislocations
$\dot{\rho}_{SSD}^{(\alpha)} = \dot{\rho}_{Lock}^{(\alpha)} - \dot{\rho}_{DR}^{(\alpha)} - \dot{\rho}_{Climb}^{(\alpha)}$	(3.29) – Dislocation evolution
$\dot{\rho}_{Lock}^{(\alpha)} = \frac{c_{Lock}}{b} \sqrt{\rho_F^{(\alpha)}} \dot{\gamma}^{(\alpha)}$	(3.30) – Lock formation
$\dot{\rho}_{DR}^{(\alpha)} = c_{DR} \rho_{SSD}^{(\alpha)} \dot{\gamma}^{(\alpha)}$	(3.31) – Dynamic recovery
$\dot{\rho}_{Climb}^{(\alpha)} = c_{Climb} \exp \left(-\frac{F_{Climb}}{kT} \right) \frac{ \tau^{(\alpha)} }{kT} \left(\rho_{SSD}^{(\alpha)} \right)^2 \left(\dot{\gamma}^{(\alpha)} \right)^{m_c}$	(3.32) – Climb annihilation
$\eta_{part} = \frac{\lambda_p}{b} \approx 1.6 r_p \left[\sqrt{\frac{\pi}{4\phi_p}} - 1 \right]$	(3.33) – Relative particle spacing (not used)
$\left(r_p(t, T) \right)^3 = r_{p,o}^3 + k_p(T) t$	(3.34) – Particle radius (not used)
$\phi_p = 0.15$	(3.35) – Volume fraction
$G(T) = G_0 - \frac{D_0}{\exp \left(\frac{T_0}{T} \right) - 1}$	(3.36) – Temperature dependent shear modulus

The crystal plasticity model in Table 3-3 has 12 material parameters, several elastic moduli that are functions of temperature, and the initial dislocation density on each of the 48 slip systems. These parameters were estimated by fitting the results of finite element tensile simulations to the experimental tensile data from Swindeman [45] for Grade 91, which has stress-strain curves for several temperatures and strain rates. This dataset had been used by Mooseburger [46] to calibrate an isotropic plasticity model for Grade 91. Presently, the data for the temperature of 600°C is relevant for the fatigue and creep simulations conducted in subsequent sections of this report. The elastic material parameters E and ν are fixed to the values appropriate for 600°C as

employed by the Norton-Bailey model. The temperature dependence of the shear modulus G is specified to agree with experimentally measured variations [24]. Initial ranges for some of the plasticity parameters were determined from explicit integration of the plastic slip rate equation and dislocation density equations in MATLAB. However, the interconnectedness of the parameters and their effects on the initial yield point and saturation stress suggested that additional help would be needed to isolate the values. With the goal of selecting material parameters that would match the response near the 600°C temperature, a modified version of the Genetic Algorithm (GA) was used since a brute force method would not be efficient enough when the values of several parameters must be obtained. This modified GA method was developed by [47] and adds a domain trimming functionality.

Due to the hundreds of generations and simulations performed during GADT, the computational model in WARP3D needed to be very simple and efficient. Therefore, the computational domain was chosen as a single trilinear hexahedral element with dimensions $5 \times 5 \times 5$ mm. The WARP3D crystal plasticity framework allows for multiple crystals to be modeled within a single element by using the Taylor (isostrain) assumption, where each crystal is assumed to experience the same applied incremental strain but responds with a different internal stress. The orientation of each crystal can be different, to approximate a polycrystal. Therefore, 100 orientations were sampled from a random texture and applied to the integration points in the single element. The boundary conditions of the model were specified for uniaxial tension, and 30 load steps of prescribed strain increments are applied to reach a total true strain of $\varepsilon = 0.03$ at constant true strain rate, to approximate the experimental conditions.

The GADT targets the best fit of the stress-strain curves compared to the Swindeman tensile data for: $T = 500^\circ\text{C}$ and $\dot{\varepsilon} = 6.7 \times 10^{-5} \text{ s}^{-1}$, $T = 550^\circ\text{C}$ and $\dot{\varepsilon} = 6.7 \times 10^{-5} \text{ s}^{-1}$, $T = 600^\circ\text{C}$ and $\dot{\varepsilon} = 6.7 \times 10^{-5} \text{ s}^{-1}$, $T = 600^\circ\text{C}$ and $\dot{\varepsilon} = 6.7 \times 10^{-5} \text{ s}^{-1}$, and $T = 600^\circ\text{C}$ and $\dot{\varepsilon} = 6.7 \times 10^{-5} \text{ s}^{-1}$. The parameters obtained from the GADT are reported in Table 3-4. Most of the parameters are in acceptable ranges as described in [28]. However, the activation energy F_0 and attack velocity v_s were somewhat larger than expected. These larger values seemed to be necessary to fit the proper strain rate and temperature sensitivity observed in the experimental data.

Table 3-4. Best fit material parameters obtained from GADT

Parameter	Value	Units
E	150,000	MPa
ν	0.285	dimensionless
D_0	8.75×10^5	MPa
T_0	4,800	K
G_0	60,940	MPa
ρ_0	1.852×10^6	mm^{-2}
ν_s	2.72×10^{12}	s^{-1}
F_0	6.901×10^{-16}	mJ
$\hat{\tau}_0$	621.9	MPa
p	1.0	dimensionless
q	1.0	dimensionless
c_ρ	0.2495	dimensionless
$c_\lambda \eta_{\text{part}}$	1,540	dimensionless
c_{Lock}	0.0058	dimensionless
c_{DR}	40.86	dimensionless
c_{Climb}	2.87×10^{-15}	$\text{mm}^5 \text{s}^{m_c}$
m_c	0.3259	dimensionless
F_{climb}	3.457×10^{-16}	mJ

Figure 3-1 shows the resulting stress-strain curves in tension corresponding to these material parameters obtained from the GA. The parameter set provides adequate results for the temperatures $T = 500^\circ\text{C}$, $T = 550^\circ\text{C}$ and $T = 600^\circ\text{C}$ with higher strain rate. The simulated stresses are larger than the experimental data at lower strain rates. Also, the amount of straining to the saturation point appears to be under-predicted. However, these parameters were obtained when the GA had settled into a stagnant state after 3 days of iterations where the fitness function values were remaining constant between generations. Also, the initial dislocation density in total across the 48 slip systems is about $9 \times 10^7 \text{ mm}^{-2}$ or $9 \times 10^{13} \text{ m}^{-2}$, which is a reasonable value for normalized and tempered martensitic steel [24]. Thus, the parameter values listed in Table 3-4 are employed within the crystal plasticity finite element simulations of the creep response of the 100 grain cell model reported in Section 3.2.6.

3.2.5 Nonlocal variables and effective power law exponent for grain boundary model

The granular deformation in Grade 91 due to crystal plasticity is one of the two primary mechanisms considered; the other is deformation along grain boundaries due to viscous sliding

and growth of cavities. As described in Chapter 2, the grain boundary cavitation model is driven by the stress field and creep strain rate in the neighborhood of the grain boundary. The model assumes an isotropic, viscoplastic, power-law constitutive relation within the grains. Within [12], this derivation is extended to the case of non-power-law, anisotropic crystal plasticity by determining an effective power-law coefficient B , and exponent n , at each volumetric finite element incident on a grain boundary finite element. A summary of those results, which logically extend to the case of crystal plasticity combined with diffusional creep in Section 3.3.2, are provided here.

The suite of isotropic viscoplastic/diffusion models of cavity/cell/grain boundary evolution is based on grain boundary and surface diffusion, coupled with an isotropic power-law viscous representation of matrix flow according to equation (3.58) in Table 3-8, where constitutive parameters are B and the power-law exponent n . The grain boundary cavitation models of [48] [49] [50] exhibit parametric dependence on n especially, as well as on the ratio $\sigma_e / \dot{\epsilon}_e^C$. When adapting anisotropic models of crystal plasticity in the grains to such models of grain boundary cavitation, it becomes necessary to make appropriate generalizations to recover “effective” values for n and B .

Table 3-5. Equations for Mises stress formulation of effective power law

Equation	Eqn. Number
$\dot{\epsilon}_e^C = B(\sigma_e)^n$	(3.37) – Power-law viscous form
$\sigma_e = \sqrt{\frac{3}{2} \boldsymbol{\sigma}' : \boldsymbol{\sigma}'}$	(3.38) – Equivalent tensile stress
$\boldsymbol{\sigma}' \equiv \boldsymbol{\sigma} - \frac{1}{3} \text{Tr} \boldsymbol{\sigma}$	(3.39) – Cauchy stress deviator
$\dot{\epsilon}_e^C = \sqrt{\frac{2}{3} \dot{\epsilon}^C : \dot{\epsilon}^C}$	(3.40) – Equivalent creep strain rate
$\dot{\epsilon}^C = \dot{\epsilon}^D + \sum_{\alpha=1}^{N_{\text{slip}}} \dot{\gamma}^{\alpha} (\mathbf{m}^{\alpha} \otimes \mathbf{n}^{\alpha})_S$	(3.41) – Combined viscoplastic strain-rate
$(\mathbf{m}^{\alpha} \otimes \mathbf{n}^{\alpha})_S \equiv \frac{1}{2} [\mathbf{m}^{\alpha} \otimes \mathbf{n}^{\alpha} + \mathbf{n}^{\alpha} \otimes \mathbf{m}^{\alpha}]$	(3.42) – Deviatoric Schmid dyadic

We focus on cubic crystals. At elevated temperatures, their viscoplastic response exhibits only limited anisotropy (for example, a lower-symmetry hexagonal crystal generally is much more anisotropic), so it seems reasonable to extract isotropic-equivalent “effective” creep properties for the single crystal, based on the viscoplastic flow rule expressed in the crystal frame according to (3.59). Therein, the flow on crystallographic slip-system ‘ α ’ is characterized by the (symmetrized) deviatoric Schmid dyadic $(\mathbf{m}^{\alpha} \otimes \mathbf{n}^{\alpha})_S$ based on slip direction $\mathbf{m}^{\alpha}$ and the slip-plane normal $\mathbf{n}^{\alpha}$, and slip-system viscoplastic shearing rate $\dot{\gamma}^{\alpha}$. Anticipating the constitutive model de-

velopments in Section 3.3.2, the combined viscoplastic strain rate is a sum of the rates due to crystal-based dislocation motion and due to diffusional creep, signified by $\dot{\epsilon}^D$.

The functional form for the slip-rate $\dot{\gamma}^\alpha = f(\tau^\alpha; \nu)$ is expressed in terms of the resolved shear stress $\tau^\alpha \equiv \boldsymbol{\sigma} : (\mathbf{m}^\alpha \otimes \mathbf{n}^\alpha)$ and a set of internal state variables (typically, dislocation densities on various slip systems), here collectively denoted ‘ ξ ’ similarly to Section 3.2.2. At any stage of the continuum crystal viscoplasticity calculations, it is clear that both $\boldsymbol{\sigma}'$ and $\dot{\epsilon}^C$ can be defined as given by (3.38) and (3.40); hence, so can σ_e and $\dot{\epsilon}_e^C$ and their quotient.

The more challenging interpretation is the (instantaneous) effective isotropic power-law creep exponent n . Note that the power-law model can be expressed by

$$\log \dot{\epsilon}_e^C = \log B + n \log \sigma_e, \quad (3.43)$$

or in terms of a strain-rate-sensitivity, with constant B ,

$$d(\log \dot{\epsilon}_e^C) = n d(\log \sigma_e). \quad (3.44)$$

Re-arranging and using the functional form of the logarithmic derivative $d(\log y) / dx = (1/y) dy / dx$,

$$n_{\text{eff}} = \frac{\sigma_e}{\dot{\epsilon}_e^C} \frac{d(\dot{\epsilon}_e^C)}{d\sigma_e}. \quad (3.45)$$

In the isotropic case, with $\boldsymbol{\sigma}'$ coaxial with $\dot{\epsilon}^C$, the creep exponent relates changes in the *magnitude* of the creep rate (proportional to $\dot{\epsilon}^C$) to corresponding changes in the magnitude of the stress deviator (proportional to $\boldsymbol{\sigma}'$). This interpretation of ‘magnitude sensitivity’ will be retained in the interpretation of an effective creep exponent for the crystal plasticity.

A straight-forward interpretation along such lines lies in taking a small assumed proportional change in the stress deviator components:

$$\boldsymbol{\sigma}^{\hat{A}}(z) \equiv (1+z) \boldsymbol{\sigma}', \quad (3.46)$$

where z is a dimensionless number that will ultimately be set to zero, leading to equivalent stress measure

$$\sigma_e^{\hat{A}}(z) = \sqrt{\frac{3}{2} \boldsymbol{\sigma}^{\hat{A}}(z) : \boldsymbol{\sigma}^{\hat{A}}(z)} = |1+z| \sigma_e, \quad (3.47)$$

and to ‘starred’ resolved shear stress measures $\tau^{\alpha;\hat{A}} = (1+z)\tau^\alpha$. The starred resolved shear stresses generate the ‘starred’ slip-system shearing rates

$$\dot{\gamma}^{\alpha;*} = f(\tau^{\alpha;*}; \xi), \quad (3.48)$$

a ‘starred’ combined viscoplastic strain rate

$$\dot{\epsilon}^* = \dot{\epsilon}^{D*}(\sigma^*(z)) + \sum_{\alpha=1}^{N_{\text{slip}}} \dot{\gamma}^{\alpha;*} (\mathbf{m}^\alpha \otimes \mathbf{n}^\alpha)_S, \quad (3.49)$$

and a ‘starred’ equivalent creep strain rate

$$\dot{\epsilon}_e^* = \sqrt{\frac{2}{3} \dot{\epsilon}^* : \dot{\epsilon}^*}. \quad (3.50)$$

The derivative of the effective creep strain rate with respect to stress can be interpreted as:

$$\frac{d\dot{\epsilon}_e^C}{d\sigma_e} = \frac{d\dot{\epsilon}_e^*}{d\sigma_e^*} \bigg|_{z=0} = \frac{d\dot{\epsilon}_e^*}{dz} \bigg|_{z=0} / \frac{d\sigma_e^*}{dz} \bigg|_{z=0}. \quad (3.51)$$

The denominator of this extended fraction, evaluated at $z = 0$, is simply $d\sigma_e^{\hat{A}}/dz = \sigma_e$. A formal treatment of the numerator is

$$\begin{aligned} \frac{d\dot{\epsilon}_e^*(z)}{dz} &= \frac{1}{2} \frac{1}{\dot{\epsilon}_e^*} 2 \frac{2}{3} \dot{\epsilon}^* : \frac{d\dot{\epsilon}^*}{dz} \\ &= \frac{2}{3\dot{\epsilon}_e^*} \dot{\epsilon}^* : \left[\frac{d\dot{\epsilon}^{D*}}{d\sigma_e^*} \frac{d\sigma_e^*}{dz} + \sum_{\alpha=1}^{N_{\text{slip}}} \frac{\partial f(\tau^{\alpha;*}; \xi)}{\partial \tau^{\alpha;*}} \frac{d\tau^{\alpha;*}}{dz} (\mathbf{m}^\alpha \otimes \mathbf{n}^\alpha)_S \right] \\ &= \frac{2}{3\dot{\epsilon}_e^*} \dot{\epsilon}^* : \left[\frac{d\dot{\epsilon}^{D*}}{d\sigma_e^*} \frac{d\sigma_e^*}{dz} + \sum_{\alpha=1}^{N_{\text{slip}}} \tau^\alpha \frac{\partial f(\tau^{\alpha;*}; \xi)}{\partial \tau^{\alpha;*}} (\mathbf{m}^\alpha \otimes \mathbf{n}^\alpha)_S \right]. \end{aligned} \quad (3.52)$$

Evaluating at $z = 0$ to obtain the derivative yields

$$\frac{d\dot{\epsilon}_e^C(z)}{dz} \bigg|_{z=0} = \frac{2}{3} \frac{\dot{\epsilon}^C}{\dot{\epsilon}_e^C} : \left[\frac{d\dot{\epsilon}^D}{d\sigma_e} \sigma_e + \sum_{\alpha=1}^{N_{\text{slip}}} \tau^\alpha \frac{\partial f(\tau^\alpha; \xi)}{\partial \tau^\alpha} (\mathbf{m}^\alpha \otimes \mathbf{n}^\alpha)_S \right]. \quad (3.53)$$

Combining equations (3.45), (3.48), and (3.49), the suggested form for 'equivalent' viscoplastic rate-sensitivity is

$$n_{\text{eff}} = \frac{2 \dot{\epsilon}^C}{3 \dot{\epsilon}_e^C} \cdot \left[\frac{d\dot{\epsilon}^D}{d\sigma_e} \frac{\sigma_e}{\dot{\epsilon}_e^C} + \sum_{\alpha=1}^{N_{\text{slip}}} \frac{\partial f(\tau^\alpha; \xi)}{\partial \tau^\alpha} \frac{\tau^\alpha}{\dot{\epsilon}_e^C} (\mathbf{m}^\alpha \otimes \mathbf{n}^\alpha)_S \right]. \quad (3.54)$$

Note that the partial derivative $\partial f(\tau^\alpha; \xi) / \partial \tau^\alpha$ is readily defined for the crystal plasticity model and is already calculated in the WARP3D code using equation (3.19). Therefore, this definition (3.54) for the effective exponent can be easily evaluated. The effective rate coefficient follows as:

$$B_{\text{eff}} = \dot{\epsilon}_e^C / (\sigma_e)^{n_{\text{eff}}} \quad (3.55)$$

These formulas (3.54) and (3.55) have been inserted into the crystal plasticity module described in Section 3.3.2 and are computed after the convergence of the local Newton-Raphson iterations to solve the coupled stress and hardening update equations (3.12) – (3.13).

Possible issues arise from this approach for determining an effective exponent. For example, the crystal plasticity model exhibits primary-like creep due to the dislocation evolution equations; incorporation of particle coarsening relations could introduce tertiary-like creep effects as well. Hence, the corresponding values of rate sensitivity can evolve during the simulation (in contrast to the assumed-constant rate sensitivity parameter n of the isotropic formulation). In simulations of creep using the 3D cell model reported in this section, constant (hard-coded) values have been assigned to the effective exponent and coefficient within the crystal plasticity subroutine: $n_{\text{eff}} = 5.0$ and $B_{\text{eff}} = 4.0 \times 10^{-18} \text{ MPa}^{-n_{\text{eff}}} \cdot \text{h}^{-1}$. These values do not affect the stress update of the CP model; they are used solely in the nonlocal variable passing scheme for the interface elements modeling cavity growth. Also, the calculations are stable for the multi-mechanism model developed in Section 3.3.2, as an example demonstrates in Section 3.4.4.

3.2.6 Modeling creep response using 3D cell model and multi-dislocation density-based model

Similar to the previous report [12], the primary benchmark case for evaluating the performance of the crystal plasticity model for creep response is the 100 grain cell model discussed in Chapter 2 for the Norton-Bailey model. This model is also employed for the simulations with the multi-mechanism crystal plasticity model described in Section 3.3.2 as well as for the final calibrations and sensitivity studies in Section 6. Therefore, the description of the cell model is repeated below, with the few distinguishing features highlighted. Additionally, key results from the multi-dislocation model described in Section 3.2.4 are reproduced from [12] to highlight proficiencies and deficiencies in the model predictions that prompted the constitutive formulation revisions in Section 3.3.2.

The 3D cell model is a $(0.2 \text{ mm})^2$ cube-shaped domain containing 100 grains that is meshed with 10,402 quadratic tetrahedral finite elements. Figure 3-2 shows the arrangement of the grains within the cell. For the CP model, the crystallographic orientation of each grain needs to be specified. The list of 100 orientations sampled from a uniform texture that is employed for the tension and fatigue simulations is also used for the cell model. As shown in Figure 3-2, all of the finite elements within the same geometric region corresponding to a grain are assigned the same Euler angles, according to the Kocks convention.

Two instances of the microstructure are considered. In the first, full continuity of the displacement field is enforced between grains in the model, to focus solely on the creep response predicted from the crystal plasticity model of dislocation climb-glide. This finite element mesh contains 15,761 nodes, which is fewer than the models in Chapter 2 because the nodes along grain boundaries have not been duplicated. In the second, 3,921 interface elements are inserted between the boundaries of the grains, leading to 25,299 nodes in the model identical to the finite element meshes analyzed in Chapter 2, and the grain boundary behavior was specified as sliding plus cavity growth but nucleation was suppressed.

The boundary conditions on the cell consist of symmetry conditions on the faces $x = 0$, $y = 0$, and $z = 0$. The effectively incomplete periodic boundary conditions obtained through multi-point constraints (MPC) are applied on the other 3 faces of the cube. For the simulations herein, a uniform pressure is applied on the $z = 0.2 \text{ mm}$ face to represent the tensile creep loading. The stress is increased linearly during 100 steps at 3.6 seconds per step to reach maximum load at 0.1 hours. This stress increase period is subsequently referred to as the “load ramp period”. The values of stress are set to 100, 120, and 140 MPa to correspond to the load levels investigated experimentally by Kimura et al. [23]. The temperature is set to 600°C. The evolution of the dislocation density state variables within the crystal plasticity model are expressed through stiff differential equations. Therefore, small time step sizes were required to achieve convergence of the nonlinear finite element equation solver. Table 3-6 lists the time steps for the simulations.

Table 3-6: Description of time steps within CP finite element simulation of creep.

Ending step	Number of steps	Time step (s)	Total model time (hr)
100	100	3.6	0.1
160	60	36	0.7
200	40	360	4.7
400	200	720	44.7
600	200	1,440	124.7
800	200	2,880	284.7
1,000	200	5,760	604.7
1,200	200	11,520	1,244.7
1,400	200	23,040	2,524.7
1,600	200	46,080	5,084.7
1,800	200	92,160	10,204.7
4,000	2000	92,160	11,2604.7

For the crystal plasticity (CP) model, material parameters identified through the genetic algorithm listed in Table 3-4 are used for the simulations of both grain deformation only and combined grain boundary deformation. The primary units are: stress, MPa; length, mm; time, seconds. The material parameters for the grain boundary cavitation model, listed in Table 3-7, were calibrated in [12] such the Norton-Bailey finite element simulation of the 3D cell model at 120 MPa and 600°C produces the same tertiary creep response as the experimental data reported by Kimura et al. [23].

Table 3-7. Material parameters for traction-separation rate equations and units

Property	Value	Units
η_b	3.6×10^5	$\text{MPa} \cdot \text{s} \cdot \text{mm}^{-1}$
a_0	0.0005	mm
b_0	0.005	mm
D	4.444×10^{-19}	$\text{MPa}^{-1} \cdot \text{s}^{-1} \cdot \text{mm}^3$
ψ	$15\pi/36$ ($= 75^\circ$)	radians

These simulations are performed on a high-performance Linux cluster with compute nodes having 20 cores with 3.1 GHz clock speed. Each of the simulation cases requires different lengths of wall time for analysis completion. For the CP model simulation with cavity growth suppressed and sliding enabled, a typical simulation with 1300 load steps required 13 hours to complete using eight cores. The statistics reported by the WARP3D output file indicate that 80% of the wall time is spent within stress updates for the crystal plasticity model. As shown in Section 3.4.1, changes to the low-level subroutines of the CP code within the past year have substantially decreased the run time.

First, three creep simulations are conducted at the applied stress levels of 100 MPa, 120 MPa, and 140 MPa for the CP only microstructural cell model. Similar to the studies for the Norton-Bailey model, the macroscopic average creep rate is computed using a finite difference calculation of the vertical nodal displacement of the top face of the cube from load step to load step. Figure 3-3 shows the variation of the creep rate during the simulation for each stress level. To more clearly interpret the response of the cell, the response of the cell model during the first 10 hours is plotted on a larger set of axes in Figure 3-3 (a), and the response under the constant applied stress is shown in Figure 3-3 (b).

During the load ramp period, the strains developed in the cell remain essentially elastic because the applied stress is below the yield stress of the material at this strain rate (approximately $1.0 \times 10^{-2} \text{ hr}^{-1} \approx 2.8 \times 10^{-6} \text{ s}^{-1}$). Thus, the observed strain rate is the elastic strain rate, which is proportional to the applied stress. After the maximum remote stress is reached at 0.1 hour, the strain rate immediately drops to the viscoplastic strain rate level corresponding to the CP equations. These strain rates exhibit a variation with applied stress, due to the exponential nature of the flow rule. Also, the 140 MPa simulation reaches a minimum creep rate after about 20,000 hours, indicating that the CP model captures the effects of both transient and steady state creep. However, the contribution observed for grain boundary sliding in Chapter 2 is typically larger than the reduction in creep rate shown in Figure 3-3 (b). Here, the creep rate drops by a factor of 10 over the duration from 10 hours to 10,000 hours. More importantly, the stress dependence of the CP model under-predicts the variation in the experimental data [23]. This discrepancy may be due to missing features in the proposed model, such as the trapping of mobile or free dislocation density within subgrain structures that lead to slowly decreasing rates of plastic strain during transient creep.

The second set of creep simulations incorporates the grain boundary mechanisms of sliding and cavity growth. Figure 3-4 shows the results for creep strain rate as a function of time for the imposed stress levels of 100, 120, and 140 MPa. The accuracy of the crystal plasticity model is quite striking for the 120 MPa load level, for which the interface material parameters were calibrated. While the minimum creep rate is overpredicted by a factor of 5, the time to minimum creep rate is much closer, at about 1,000 hours compared to 2,000 hours in the experimental data. The computed solution is also reasonable for the 140 MPa stress level. However, the creep strain rate for 100 MPa is overpredicted during much of the simulated creep lifespan, and the simulated strain rate variation is less compared to the experimental data. Each of the computed strain-rate curves appear flatter than the corresponding measured curves, meaning that less evolution of the microstructure is captured in the model during early creep life. As indicated by the results for the CP-only model, the characterized stress-dependent features of the crystal plasticity material flow rule require modification to capture this variation correctly.

The overall trends shown in Figure 3-4 indicate that the current CP model overpredicts the creep strain rates experienced within the 3D cell model. These preliminary results are impacted

by several factors. First, the crystal plasticity material parameters are calibrated to match the stress-strain curves for older specimens of Grade 91 tested by Swindeman [45]. Second, the finite element models used for the calibration process contain only one solid element where the grains are approximated using the isostrain assumption. Third, the material parameters for the grain boundary constitutive models as well as the NB model for the grains are calibrated together to match the minimum creep rate and tertiary response of the experimental data from Kimura et al. [23]. Nonetheless, an extensive study of different material parameter sets for the crystal plasticity and interface constitutive models did not produce an improved fit to the experimentally observed primary creep behavior while simultaneously matching the tensile stress-strain curves from Swindeman [45]. This discrepancy suggested that a different creep deformation mechanism is active at the lower stress levels that is not captured in the proposed model in Section 3.2.4, thereby prompting the investigation of the multi-mechanism model in Section 3.3.2.

3.3 Crystal plasticity algorithmic platform and multi-mechanism constitutive model

Building from the crystal plasticity finite element platform in Section 3.2.2, the mechanisms for dislocation creep and diffusional creep outlined in Section 3.1 have been incorporated into the framework. This section describes these components and the calibration of the constitutive parameters used in both deformation mechanisms. Subsequently, parametric studies are performed in Section 3.4 to understand the relative effects of specific material parameters, plastic anisotropy arising from dislocation creep, and fraction of creep strain due to diffusional creep.

3.3.1 Algorithmic platform for crystal plasticity in WARP3D

Following the extension of the crystal plasticity subroutines in WARP3D to allow multiple hardening variables, several inefficiencies were observed in the code that detracted from the method's performance. These factors have been improved during the past year and are documented below.

Many crystal plasticity constitutive models require the value of plastic slip rate $\dot{\gamma}^{(s)}$ in multiple equations. Within the code, these slip rates were recomputed several times rather than computed a single time and stored in local memory. Now, the slip rates are calculated less frequently and instead stored in local memory. Also, other coding inefficiencies have been corrected which before had led to creation of temporary arrays and other unneeded overhead. These revisions provide a factor of speed up between 8 and 20.

For the previous report term, a bookkeeping system of indices was created in order to reference the various quantities in the history vector. This revision facilitates adding new features and simplifies the output of state variables to text files at the completion of load steps. The bookkeeping system was verified through extensive testing between four types of crystal plasticity models and slip systems to ensure that the conversion of the implementation was seamless. Also, the FORTRAN package for nonlinear equation solving, "nleqslv" developed by Hasselman [29], was incorporated into the material subroutine. This package contains both Newton and Broyden Se-

cant method nonlinear equation solvers with line search and trust region modules. These solution techniques helped to improve the robustness of the material subroutine.

This reporting period, the bookkeeping system for the history vector was expanded to account for the pseudo diffusion model described in Section 3.3.2. The existing Voce crystal plasticity model in WARP3D was revised to use a constant pre-factor in the power-law expression also described in the following section. Also, the nonlocal variable sharing for from the crystal plasticity solid elements to the grain boundary interface elements was verified through a series of small benchmark tests as well as calculations for the 100 grain cell model. Several other modifications to the code were made in regards to other constitutive models. Lastly, a verification suite of input files was developed to cover most of the functionality in the crystal plasticity subroutine, which includes the models described in Sections 3.2 and 3.3.

With these changes, the crystal plasticity model in WARP3D now contains over 27,000 lines of code in comparison to less than 4,000 lines in 2013 prior to commencing the efforts described in this report. Listings of the file sizes are given below.

- mod_crystal.f, 2508 lines, previously 936 lines
- mm10.f, previously 3463 lines
- mm10_a.f, 4029 lines: routines for driving the stress update equations, routine for quadrature point output quantities, and other utilities
- mm10_b.f, 5855 lines: routines for constitutive models
- mm10_c.f, 5911 lines: routines from solver package “nleqslv” and interfacing scripts
- mm10_d.f, 475 lines: routine for history variable bookkeeping
- mm10_e.f, 6295 lines: lists of hard-coded values for interaction matrix coefficients
- mm10_f.f, 2052 lines: routines to support various states output options

3.3.2 Multi-mechanism model for creep deformation in prior austenite grains

Several revisions to the mechanism-based crystal plasticity constitutive equations were accomplished during the past year. While some positive features were exhibited by the multi-dislocation density-based model in Section 3.2.4, several drawbacks of this model were also identified. First, the simulated creep curves did not capture the long duration of primary creep exhibited in the experimentally measured response, which could affect the history of stress concentrations at triple points and grain boundaries that lead to the eventual acceleration of creep strain rate. Second, the stress-sensitivity of the model was less than the measurements of Grade 91, so that the differences of minimum creep strain rate were not well approximated at load levels other than 120 MPa in Figure 3-4. Third, experimental data for minimum creep strain rate obtained by Kloc et al. [27] exhibit a change in deformation mechanism at applied stress below 100 MPa at 600 C. Figure 3-6 shows the variation of minimum strain rate for different stresses from two

Grade 91 creep test data sets; other sources show similar trends with power law relationship with $n = 1$ below 100 MPa and $n > 10$ above 100 MPa. Fourth, the previous model contained hardening variables representing the dislocation density on each of the 48 BCC slip systems. Several studies, such as Section 3.4.3, indicated that the local anisotropy of the crystal plasticity model did not have a significant effect on the bulk response of the cell model during creep simulations. Without local stress or strain measurements of crystal-scale deformation during creep tests, the added computational expense from tracking many state variables at each integration point was difficult to justify.

In pursuit of understanding the deformation mechanism transition in Grade 91 at lower operating stresses at temperatures at or below 600 C, a multi-mechanism crystal plasticity model is proposed in equation (3.56) that is a combination of dislocation creep (3.57) and diffusional creep (3.58). These two mechanisms, described subsequently, are assumed to occur simultaneously through motion of different types of defects (dislocations and atoms/vacancies), and thus the strain rates from each are summed together.

Table 3-8. Combined mechanisms of crystallographic viscoplastic flow and diffusional creep for Grade 91 constitutive model

Equation	Number
$\dot{\mathbf{t}} = \mathbf{C}_o : (\mathbf{d} - \bar{\mathbf{d}}^p - \mathbf{d}^d) + \mathbf{R}\bar{\mathbf{w}}^p \mathbf{R}^T \mathbf{t} - \mathbf{t} \mathbf{R}\bar{\mathbf{w}}^p \mathbf{R}^T$	(3.56) – Unrotated Cauchy stress update
$\bar{\mathbf{d}}^p = \sum_{s=1}^{n_{slip}} \dot{\gamma}^{(s)} \mathbf{R}^{pT} \tilde{\mathbf{m}}^{(s)} \mathbf{R}^p$	(3.57) – Plastic strain rate
$\mathbf{d}^d = D_\eta(T) \text{dev}(\mathbf{t})$	(3.58) – Diffusional strain rate
$\dot{\gamma}^{(s)} = \frac{\dot{\tilde{\gamma}}}{\tilde{\tau}} \left \frac{\tau^{(s)}}{\tilde{\tau}} \right ^{n-1} \tau^{(s)}$	(3.59) – Power-law slip rate
$\tilde{\tau} = \tau_y + \tau_w$	(3.60) – Slip resistance
$\dot{\tau}_w = \theta_0 \left(1 - \frac{\tau_w}{\tau_v} \right)^m \sum_{s=1}^{n_{slip}} \dot{\gamma}^{(s)} $	(3.61) – Hardening rate
$D_\eta(T) = D_{\eta 0} \exp(-Q_\eta/kT)$	(3.62) – Diffusional creep coefficient

Table 3-9. Nomenclature for Grade 91 model and physical units employed

Property	Description	Units
$\dot{\gamma}^{(s)}$	Plastic slip rate	s^{-1}
$\dot{\bar{\gamma}}$	Reference strain rate	s^{-1}
$\tau^{(s)}$	Resolved shear stress	MPa
$\tilde{\tau}$	Mechanical slip resistance	MPa
τ_y	Initial flow resistance	MPa
τ_w	Immobilizing flow resistance	MPa
τ_v	Saturation stress	MPa
n	Flow rule power law exponent	dimensionless
θ_0	Flow curve modulus	MPa
m	Shape factor	dimensionless
D_η	Diffusional constant for linear viscous flow	$MPa^{-1} \cdot s^{-1}$
$D_{\eta 0}$	Reference diffusion coefficient	$MPa^{-1} \cdot s^{-1}$
Q_η	Activation energy	Joules
k	Boltzmann constant	$J \cdot K^{-1}$

To represent dislocation creep according to the climb plus glide mechanism, a power-law expression (3.59) is adopted for the slip rate $\dot{\gamma}^{(s)}$ on each of the 12 primary $\{110\}\langle\bar{1}11\rangle$ BCC slip systems. A variant of this model existed in prior version of WARP3D [14] and was adjusted to have a constant pre-factor slip rate $\dot{\bar{\gamma}}$. Taylor hardening is assumed such that the drag stress or slip resistance $\tilde{\tau}$ is equal for each slip system, and the strengthening portion of the resistance τ_w evolves according to a Voce equation (3.61). This model can account for either softening (decrease) or hardening (increase) of the slip resistance by specifying negative or positive values, respectively, of the saturation stress τ_v and flow modulus θ_0 . Studies for each parameter's effect on the cell model creep response are presented in Section 3.4.2.

The diffusional creep mechanism that is dominant at lower applied stress is represented through a linear viscous equation (3.58) in terms of the deviatoric part of the stress tensor and a generic diffusion coefficient expressed by an Arrhenius relation (3.62). The diffusion constant is assumed to be independent of time and the strain history. Diffusional creep in simple polycrystalline materials, such as pure metals with limited solid solution strengthening, are traditionally categorized as one of three classes of mechanisms: Nabarro-Herring creep [51], Coble creep [52], and Harper-Dorn creep [53]. The term Nabarro-Herring creep corresponds to diffusion of atoms or vacancies through the lattice of grains due to differentials in deviatoric stress across the grain, while Coble creep refers to their diffusion along grain boundaries; the exact nature of Harper-Dorn creep is still disputed [54]. The key factors for differentiating among this set of idealizations are the grain-size dependence of creep rate at fixed temperature and stress, and the relative values of inferred activation energies based on creep rates at the same stress but differing temperatures within a particular regime. The complexity of microstructures in quenched and tempered

martensitic steels like Grade 91, which possess features at several length scales, has complicated the delineation of these mechanisms such that the literature has generally refrained from making definitive categorizations of the linear viscous/diffusional creep mechanisms in Grade 91.

The isotropic linear viscous grain deformation term is a simplification of the likely physical mechanisms occurring in the material. When dislocation motion within the grain is the mechanism, local deviatoric stress does provide the driving force in terms of a resolved shear stress on the slip system, but in any diffusional mechanism, the key idea is that there is a lattice flux of mass (atoms going one way, or, equivalently, vacancies going the other), with “sources” and “sinks” marking the beginnings and endings of the respective lattice journeys. The difference in chemical potential between the endpoints provides the driving force; usually the endpoints are taken to lie on internal (or external) interfaces such as grain boundaries, and a major part of the driving force is the normal stress on the boundary. Atomic diffusion proceeds from lower-normal-stress boundaries toward higher-normal-stress boundaries, where the plating out effectively allows the energy of the system to lower. Vacancy diffusion proceeds in the opposite direction, effecting the same results. Deviator stress within a given grain does lead to differing normal stress on its respective grain boundary segments, so that the spirit of the geometrical effects of diffusion are reflected through the linear viscous strain-rate term, and the cell-averaged deformations collect these responses in an essentially correct accounting. However, the local effects of atomic diffusion on and near the grain boundaries (above and beyond those associated with cavity nucleation and growth) are not followed in detail.

Nonetheless, these quenched and tempered alloys have very high dislocation densities and very small grain/subgrain sizes, especially when contrasted with more traditional larger-grain-size creep-resistant alloys. Both of these microstructural features can enhance effective atomic diffusivity: “pipe diffusion” along dislocation cores, and boundary diffusion at grain/subgrain interfaces. Thus, there are good reasons to expect important roles of diffusional deformation in these materials, even at lower homologous temperatures than typically associated with “dominant” diffusional mechanisms. The use of linear viscous (isotropic) deformation in the grains is one way to account at certain larger scales for whatever detailed diffusional mechanisms are operative. Further investigation of these mechanisms using smaller length scale models is particularly warranted.

3.3.3 *Estimation of Voce power-law material parameters*

The final set of calibrated material parameters for the power-law dislocation creep model were determined by fitting the creep response of the 3D cell model to experimental data. However, the determination of some model parameters could be made from simpler calculations. The recorded minimum strain rates from the Grade 91 tests by Kimura et al. [23] at 600 C are presented in Figure 3-7, and the least-squares fit linear trend line is given as well. The slope of the line is 11.78, suggesting that the power-law exponent for the flow rule (3.59) dominant at higher stresses should be set to $n = 12$. The constant coefficient of the trend line is about $6.56 \times 10^{-31} \text{ hr}^{-1}$, which is a combination of the pre factor $\dot{\gamma}$ and slip resistance $\tilde{\tau}$. Comparing other crystal plasticity constitutive models for Grade 91 [32] [55] suggested that a reasonable value for the slip resistance is $\tilde{\tau} = 40 \text{ MPa}$. Thus, this value was assigned to τ_y in a single finite element with single crystal orientation having Kocks Euler angles $(\Psi, \Theta, \varphi) = (0, 90, 45)$, subjected to a constant

strain true rate of $8.52 \times 10^{-7} \text{ hr}^{-1}$. The value of $\dot{\gamma}$ was then adjusted until the axial stress of the finite element saturated at 110 MPa, which corresponds to the data in Figure 3-7. The resulting value of $\dot{\gamma} = 9.55 \times 10^{-8} \text{ hr}^{-1}$ was subsequently employed during all later simulations of the 3D cell model creep studies in Chapter 6.

Direct comparisons of the Voce power-law model with the Norton-Bailey isotropic creep model studied in Chapter 2 were also desired. Thus, a similar tension test except using an iso-strain model with 100 crystal orientations was performed at a strain rate corresponding to 120 MPa. The resulting parameters are $n = 5$, $\dot{\gamma} = 6.5 \times 10^{-8} \text{ hr}^{-1}$, $\tau_y = 40 \text{ MPa}$, and $\tau_v = 0$.

3.3.4 Estimation of diffusional creep parameters

The calibration of the diffusional creep coefficient (3.58) was performed for stresses below 60 MPa, where this mechanism is expected to be active. The measured minimum creep strain rates at different applied stresses from Kloc [27] for Grade 91 are taken as a reference dataset for calibration. They report results from three different temperatures: 873 K, 923 K, and 973 K. We therefore calibrate both the stress and temperature dependence of the diffusional creep rate. At these low stress levels, the dislocation creep term is assumed to be negligible. Also, the constitutive relation is a function of the deviatoric stress and does not contain crystallographic or hardening terms. Therefore, a model with a single finite element is sufficient for calibrating the material parameters for the behavior after all grain boundary sliding has reached equilibrium.

Figure 3-8 shows the creep strain rate versus applied stress for the experimental data as symbols compared with the numerical curves from the best-fit parameters. The MATLAB optimization function “fminsearch” was employed to minimize the distance between the experimental and numerical curves at each temperature, with a higher weight applied to the 873 K data because this temperature is the focus of subsequent model studies. The resulting parameters are $D_{\eta_0} = 1.52 \times 10^{-7} \text{ MPa}^{-1} \cdot \text{s}^{-1}$ and $Q_{\eta} = 1.45 \times 10^{-19} \text{ J}$, yielding a diffusion coefficient of $D_{\eta} = 9.19 \times 10^{-13} \text{ MPa}^{-1} \cdot \text{s}^{-1}$ at 873 K, which are reasonable values for diffusion and activation energy. These values are taken as a starting point for the combined calibration studies in Chapter 6 for the combined grain and grain boundary models.

3.4 Crystal plasticity simulation of creep using 3D cell model

The most important assessment of the performance of the multi-mechanism crystal plasticity model is its ability to model the response of Grade 91 under creep conditions. Therefore, these investigations align with the primary objective of creep life extrapolation for in-service conditions using a physically-based model. Similar to the previous report [12], the primary benchmark case for evaluating the performance of the crystal plasticity model for creep response is the 100 grain cell model discussed in Chapter 2 for the Norton-Bailey model. This model is also employed for the simulations with the multi-mechanism crystal plasticity model described in Section 3.2.6 as well as for the final calibrations and sensitivity studies in Chapter 6.

3.4.1 3D cell model description and creep response with cavity growth suppressed

The 3D cell model is a $(0.2 \text{ mm})^2$ cube-shaped domain containing 100 grains that is meshed with 10,402 quadratic tetrahedral finite elements. Figure 3-2 (a) shows the arrangement of the grains within the cell. The crystal orientations in the 100 grains are sampled from a uniform texture. The microstructure model contains 3,921 interface elements and 25,299 nodes in the model identical to the finite element meshes analyzed in Chapter 2, and the grain boundary behavior was specified as sliding plus cavity growth but nucleation was suppressed.

The boundary conditions on the cell consist of symmetry conditions on the faces $x = 0$, $y = 0$, and $z = 0$. The effectively incomplete periodic boundary conditions obtained through multi-point constraints (MPC) are applied on the other 3 faces of the cube. For the simulations herein, a uniform pressure is applied on the $z = 0.2 \text{ mm}$ face to represent the tensile creep loading. The stress is increased linearly during 10 steps at 0.01 hours per step to reach maximum load at 0.1 hours. This stress increase period is subsequently referred to as the “load ramp period”. The values of stress are set to 100, 110, 120, 140, and 160 MPa to correspond to the load levels investigated experimentally by Kimura et al. [23]. The temperature is set to 600°C. The evolution of the internal state variables within the crystal plasticity model is expressed through stiff differential equations. Therefore, small time step sizes were required to achieve convergence of the nonlinear finite element equation solver. Table 3-10 lists the time steps for the simulations.

Table 3-10: Description of time steps within CP finite element simulation of creep.

First series step	160 MPa	140 MPa	120 MPa	110 MPa	100 MPa
1	0.01	0.01	0.01	0.01	0.01
11	0.04	0.05	0.07	0.08	0.1
101	0.06	0.08	0.126	0.152	0.2
201	0.09	0.128	0.2268	0.2888	0.4
301	0.135	0.2048	0.40824	0.54872	0.8
401	0.2025	0.32768	0.734832	1.042568	1.6
501	0.30375	0.524288	1.322698	1.980879	3.2
601	0.45563	0.838861	2.380856	3.763670	6.4
701	0.68344	1.342177	4.28554	7.150973	12.8
801	1.02516	2.147484	7.713972	13.58685	25.6
901	1.53773	3.435974	13.88515	25.81501	51.2
1,001	1.53773	3.435974	13.88515	25.81501	51.2
2,000	1,990.75	4,343.50	16,269.1	31,255.3	61,429.1

These simulations are performed on a high-performance Linux cluster with compute nodes having 20 cores with 3.1 GHz clock speed. Each of the simulation cases requires different lengths of wall time for analysis completion. For the CP model simulation with cavity growth suppressed and sliding enabled, a typical simulation with 2000 load steps required about hours to

complete using ten cores. This is a speed up of more than ten times compared to the simulations from the multi-dislocation density-based model [12].

Table 3-11. Material parameters for multi-mechanism crystal plasticity (CP) model

Property	Value	Units
E	150,000	MPa
ν	0.285	dimensionless
τ_y	40.0	MPa
τ_v	12.0	dimensionless
n	12	dimensionless
θ_0	800.0	MPa
m	1	dimensionless
D_η	1.2×10^{-9}	$\text{MPa}^{-1} \cdot \text{s}^{-1}$

Table 3-12. Material parameters for traction-separation rate equations and units

Property	Value	Units
η_b	1.0×10^6	$\text{MPa} \cdot \text{hr} \cdot \text{mm}^{-1}$
K_{lin}^{user}	1.0×10^8	MPa/mm

To focus on the creep behavior of the multi-mechanism crystal plasticity model, creep simulations are performed for each of the load levels with the grain boundary cavity growth terms suppressed. The set of material parameters are listed in Table 3-11 and Table 3-12, which were calibrated for the primary creep regime alone. Figure 3-9 presents the evolution of creep strain rate for the cell model at each load level. Notice that the relation of strain rate to time is closely captured for each of the load levels during the transient or primary creep regime.

The chosen parameters include both hardening in the Voce model as well as moderate sliding along grain boundaries. Previous studies [12] indicated that grain boundary sliding is necessary to facilitate cavity growth, while more recent studies conducted in Chapter 4 highlight that reasonable values for the viscosity are required for numerical stability. Also, another study in Section 6.3 shows that the inclusion of grain boundary sliding leads to slightly greater strain rates in the cell model. Thus, the combination of the viscosity and the crystal plasticity parameters were calibrated together. Nonetheless, these parameters could be found separately before adjusting the grain boundary cavity growth parameters to match the tertiary creep regime, which is an advantage of the model.

The power-law exponent of 12 for the dislocation creep model provides the correct stress-sensitivity to match the experimental data from Kimura et al. [23]. However, none of the creep curves actually reach saturation in the Voce model; each of the curves is terminated because 2000 time steps have been completed. Other sets of material parameters may also produce results that

match closely to portions of the experimental data, such as those in Section 3.4.4, but the tertiary portion of the material response is best captured with these parameters, as shown later in Section 6.2. The calibrated Voce parameters produce a hardening response, or an increase to plastic slip over time. This behavior may seem to conflict with the cyclic softening during fatigue tests and flow softening during tensile tests at high temperatures for Grade 91 [12]. The authors attribute the extended period of primary creep with decreasing strain rate at constant load to the reduction of initial mobile dislocation density that becomes immobilized against microstructural obstacles such as subgrain boundaries or precipitates. Mobile dislocation density, initially present after the material processing, is responsible for plastic strain according to the Orowan equation $\dot{\gamma} = \rho_m b v$; therefore, a reduction in mobile dislocation density fraction would lead to overall lower creep rates in the grains.

For all of the load levels 100 to 160 MPa, the maximum discrepancy in the transient strain rate is a factor of two, and the simulated and experimental creep curves overlap for much of the strain history prior to onset of tertiary creep in the measured curves.

3.4.2 Effect of dislocation creep material parameters on cell model response

Several parameter studies were conducted on the 3D cell model to understand the effect of each of the main crystal plasticity constitutive parameters on the bulk deformation of the cell: initial flow stress τ_y , saturation stress τ_v , flow curve modulus θ_0 , and rate-sensitivity exponent n .

The first study was performed using parameters calibrated to match the Norton-Bailey model in Chapter 2 for the iso-strain tensile test: $\dot{\gamma} = 6.5 \times 10^{-6} \text{ hr}^{-1}$, $\tau_y = 40 \text{ MPa}$, $n = 5$, and $m = 1$. This provides a reference point for comparing the isotropic and crystallographic creep models. Six combinations of the saturation stress and flow modulus are considered: (1) $\tau_v = 0 \text{ MPa}$, $\theta_0 = -400 \text{ MPa}$; (2) $\tau_v = -2 \text{ MPa}$, $\theta_0 = -400 \text{ MPa}$; (3) $\tau_v = -4 \text{ MPa}$, $\theta_0 = -40 \text{ MPa}$; (4) $\tau_v = -4 \text{ MPa}$, $\theta_0 = -400 \text{ MPa}$; (5) $\tau_v = -4 \text{ MPa}$, $\theta_0 = -4000 \text{ MPa}$; and (6) $\tau_v = -10 \text{ MPa}$, $\theta_0 = -400 \text{ MPa}$. The negative values of τ_v are expected to lead to softening material response, and thus increased creep strain rate at constant stress. Softening was initially investigated because most of the experimental data for tensile tests at higher strain rates exhibit flow softening, as shown in Section 3.2.4 particularly for higher temperatures at or above 600 C. The material parameters for the multi-dislocation density based model were also calibrated to exhibit softening in fatigue simulations [12]. For these simulations, the grain boundary model was incorporated with sliding and cavity growth effects but nucleation suppressed: $\eta_b = 100 \text{ MPa} \cdot \text{hr} \cdot \text{mm}^{-1}$, $a_0 = 0.0005 \text{ mm}$, $b_0 = 0.005 \text{ mm}$, $\psi = 75^\circ$, and $D = 8.0 \times 10^{-16} \text{ MPa}^{-1} \cdot \text{hr}^{-1} \cdot \text{mm}^3$. Note that these parameters are such that cavity growth starts from the beginning of the simulations.

Figure 3-10 shows the variation of average creep strain rate in the loading direction for an applied stress of 100 MPa on the 3D cell model. The flow modulus θ_0 appears to have the largest effect on the onset of tertiary creep. Other than the non-softening parameter set, the case with $\theta_0 = -40 \text{ MPa}$ has the lowest overall strain rates. Meanwhile, the simulation with

$\theta_0 = -4000$ MPa has the fastest strain rates and actually diverges before the tertiary behavior is reached. The effect of the saturation stress τ_v is somewhat different. For increasing levels of softening, the period from secondary to tertiary creep becomes more gradual, compared to the sharper curves without softening.

Another representative set of simulations were performed with grain boundary sliding suppressed $\eta_b = 1 \times 10^9$ MPa · hr · mm⁻¹ and an applied stress of 140 MPa. The Voce model parameters are set to: $\dot{\gamma} = 9.55 \times 10^{-8}$ hr⁻¹, $n = 12$, and $m = 1$. Hardening behavior of the flow stress is considered in Figure 3-11 with three different combinations of the slip resistance and saturation τ_v ; the flow modulus is fixed to $\theta_0 = 4000$ MPa. Note that the final slip resistance $\tilde{\tau} = \tau_y + \tau_v = 37$ MPa is identical for all three cases; hence, it is logical that the average strain rate of all simulations converges to the same value at long durations. Thus, the parameter $\tau_y + \tau_v$ specifies the steady state creep rate reached by the model; note that the accumulated strain at a given time instant will be different due to initial transients. Also, the lower yield stress $\tau_y = 24$ MPa produces the highest initial strain rates after the load ramp period is completed. A further alteration of the $\tau_y = 25$ MPa, $\tau_v = 12$ MPa case is performed with a reduced flow modulus $\theta_0 = 400$ MPa, and Figure 3-12 examines this effect on the history of creep strain rate at 140 MPa load level. The initial transient strain rate of both cases is fairly similar. Also, the final steady strain rate of 1×10^{-5} hr⁻¹ is the same for both cases, meaning that the modulus does not impact the final converged strain rate. However, the evolution toward the minimum rate is much faster for the larger modulus case. Note that the slope both curves during the intermediate portion of primary creep are similar through; this slope and the relative duration of constant-appearing rate of strain-rate-reduction regime are likely attributed to the shape parameter m in the Voce model.

3.4.3 Effect of spatial arrangement of crystal orientations

In this section, the influence of the spatial arrangement of grain lattice orientations on the cell average creep strain rate and the local distribution of stress is investigated. For most of the simulations in the report, a specific set of orientations from a uniform texture are assigned to the 100 grains of the cell model in an identical fashion, so that results on identical microstructures can be used to compare the effects of different material parameters and loading conditions. Therefore, knowing the sensitivity of the computed results with respect to the cell geometry and crystal orientation is important. Herein, the list of 100 orientations are assigned in five different spatial arrangements to the cell model, and the creep test at 120 MPa was conducted using the material parameters from Table 3-11 with cavity growth suppressed.

Figure 3-13 contains each of the five creep strain rate versus time curves for the different instantiations of texture in the microstructure. All curves are nearly identical, with the largest differences appearing near the end of the simulation. At time $t = 10^4$ hr, across the simulations, the maximum strain rate is 8.39×10^{-7} hr⁻¹, the minimum rate is 7.51×10^{-7} hr⁻¹, and the average is 8.01×10^{-7} hr⁻¹, indicating the difference is about 5%.

Figure 3-14 provides histograms of the Mises stress field in each element of two simulations with different spatial arrangements of orientations. The tails of the two distributions are fairly similar, while the frequencies of stresses in the intermediate levels exhibit somewhat distinct character.

Thus, the distribution of orientations had a very mild effect on the bulk cell average creep rate during the primary and secondary creep regimes. This conclusion is logical for random texture; larger sensitivity might occur in the tertiary creep regime due to the effect of stress concentrations on the local cavity growth rate. Also, changes to the grain and grain boundary geometry may induce a larger change to the cell response, such as the results for periodic microstructures presented in Chapter 5. In particular, the ratio of grain boundary surface area to grain volume within the cell model is a critical parameter to match with the experimental characterizations of Grade 91 steel. Setting the average grain diameter to be similar to the measured diameter of prior austenite grains is important to achieve an appropriate relative contribution of grain bulk GB deformation in the final model

3.4.4 Effect of grain diffusional creep at lower load levels

Determining the prominent deformation mechanisms for Grade 91 at typical operating stress is a major objective of this project. Therefore, the creep behavior of the cell model was compared when the diffusional creep term was active and inactive within the grains. These effects are isolated by suppressing cavity growth as well as grain boundary sliding. The remaining parameters in the crystal plasticity model were adjusted to closely match the experimental data from Kimura et al. [23]. The values are: $\dot{\gamma} = 9.55 \times 10^{-8} \text{ hr}^{-1}$, $\tau_y = 25 \text{ MPa}$, $n = 12$, $m = 1$, $\tau_v = 12 \text{ MPa}$, $\theta_0 = 4000 \text{ MPa}$, and $\eta_b = 1 \times 10^9 \text{ MPa} \cdot \text{hr} \cdot \text{mm}^{-1}$. Also, the simulations were conducted using an earlier version of the grain constitutive model where the diffusional creep was partitioned onto the BCC slip systems so that $\dot{\gamma}^{(s)} = \dot{\gamma}_{Voce}^{(s)} + \dot{\gamma}_{Diff}^{(s)}$ with $\dot{\gamma}_{Diff}^{(s)} = D_\gamma \tau^{(s)}$ rather than the isotropic deviator-based diffusional creep model (3.56) with the deformation rate tensor $\mathbf{d}^{vp} = \bar{\mathbf{d}}^p + \mathbf{d}^d$. The qualitative behavior of these two equations for the cell average creep strain rate are similar, but the simpler constitutive model was adopted because the diffusional deformation could not be readily justified to be linked to crystallographic directions. The value of $D_\gamma = 5.9 \times 10^{-9} \text{ MPa}^{-1} \cdot \text{hr}^{-1}$ is used herein.

Figure 3-15 and Figure 3-16 examine the evolution of the average creep strain rate as a function of time at various applied loads when diffusional creep is included and excluded, respectively. The curves at the higher stresses 140 and 160 MPa are nearly identical on the logarithmic scale. The creep rate curve for 120 MPa is somewhat higher for the diffusional creep case in Figure 3-15. The larger minimum strain rates are most evident for the lower stresses of 100 and 110 MPa. These effects on the simulated creep strain rates can be explained by considering the polynomial form of the viscoplastic flow rule (3.59). For large applied stress, the value of the polynomial x^{12} is much greater than x , but at lower stresses the linear polynomial term becomes greater. Since the two deformation modes are added together in series and the polynomial terms have different prefactors, there is expected to be a stress level where both terms have equal magnitude. The uniaxial tensile stress at which this transition is evident in the experimental data [27]

is about 100 MPa. Below this value, the slope of the curve on logarithmic scale is approximately unity.

The significant increase in the minimum creep rate at the 100 MPa load level is shown in Figure 3-17. The response of the cell models with and without the diffusional term is identical up to about 100 hours. Recall that the diffusional creep term has a constant flow resistance or diffusivity, such that the primary or transient creep regime should only be affected at later times in the simulation. The minimum strain rate is reached at about 100,000 hours. Note that cavity growth is suppressed, which delays the onset to minimum. Also, these simulations were performed with nonlinear kinematics in WARP3D in contrast to most of the other simulations in this report, which explains why the strain rate begins to increase after the minimum is reached. These accelerations occur several magnitudes of time later than the experimental data and can thus be ignored. The minimum strain rates with and without diffusional creep are $6 \times 10^{-7} \text{ hr}^{-1}$ and $2 \times 10^{-7} \text{ hr}^{-1}$ respectively, so that the diffusional mechanism accounts for about twice the flow compared to the crystallographic dislocation glide mechanism.

Figure 3-18 provides a comparison of the minimum strain rate as a function of applied stress for the two models and the experimental data from Kimura et al. [23]. The cell model response including the diffusional creep is consistently greater than the experimental data points for all stress levels while the Voce crystal plasticity model underpredicts the strain rates for the lower stresses levels. Thus, accounting for this shift in dominant mechanism is important for capturing the response of the material at service load levels.

Next, the mechanical fields within the microstructure are examined at different applied stress levels to better understand the features of the two deformation mechanisms. Several simulations of the cell model are performed, with cavity growth suppressed and free sliding, for the following stresses: 5 MPa, 10 MPa, 60 MPa, 100 MPa, 125 MPa, and 135 MPa. The material parameters are set to: $\dot{\gamma} = 2.35 \times 10^{-6} \text{ hr}^{-1}$, $\tau_y = 40 \text{ MPa}$, $n = 10$, $m = 1$, $\tau_v = 0 \text{ MPa}$, $\theta_0 = 400 \text{ MPa}$, $D_\gamma = 5.2 \times 10^{-9} \text{ MPa}^{-1} \cdot \text{hr}^{-1}$, and $\eta_b = 1 \times 10^2 \text{ MPa} \cdot \text{hr} \cdot \text{mm}^{-1}$.

Simulations were carried out for each applied stress until the cell average strain rate became saturated and no longer decreased. Then, fringe plots of the von Mises stress field in each of the finite elements of the microstructure were examined. The ratio of the maximum stress across all elements to the applied stress is taken as a measure of the strength of stress concentrations within the cell model. The value of this ratio are listed in Table 3-13. Higher stress concentrations appear for the lower applied stresses, when the diffusional creep term is dominant. Recall that the cell model simulations are traction-driven problems and the strain rate is computed. However, compatibility is enforced within the cell, so that material regions with locally higher strain rates will quickly be constrained by regions that are deforming more slowly. Then, the creep rate across the cell must be reasonably similar. Now, for larger stress exponents, a small change in stress (due to a concentration) would lead to larger strain rates that would be constrained by neighboring material. At lower exponents, a greater differential stress could be carried at a point before the strain rate increases significantly to lead to incompatibilities. This explanation appears consistent with the observed trends of stress concentration factors.

Table 3-13: Ratio of maximum von Mises stress to cell average stress

Stress (MPa)	5	10	60	100	125	135
Concentration Factor	4.1	4.1	2.4	2.2	2.1	2.1

Fringe plots of the von Mises stress field are shown for selected applied stress levels in Figure 3-19. The time of the snapshot in each simulation corresponds to the minimum strain rate. The highest local stress values appear at consistent locations for all load levels, since the crystal orientations are the same for all models as well as all material parameters. However, the gradation of contours is largest for the 10 MPa applied stress case. Also, Figure 3-20 provides fringe plots for the n_{eff} scalar field computed from the formulas developed in Section 3.2.5. Recall that n_{eff} is one of the nonlocal fields required by the cavity growth model. At the low 10 MPa stress and high 125 MPa stress, the computed exponent n_{eff} is constant across the entire cell, meaning that a single mechanism dominates everywhere. However, at 60 MPa, much of the domain exhibits $n_{eff} = 1$ while locations experiencing higher von Mises stresses exhibit $n_{eff} \geq 5$. In the actual Grade 91 material, the local stress and strain state near a cavity population on a grain boundary is what is expected to drive the cavity evolution. Therefore, capturing the heterogeneity of these fields is one benefit that the cell model provides over reduced order models that smear out the heterogeneities.

3.5 Summary of crystal plasticity modeling framework

This section summarizes the progressive developments of the crystal plasticity modeling framework for Grade 91 during this project. The constitutive equations account for anisotropic straining due to dislocation glide on preferential planes in the crystal lattice. The CP model contains terms for dislocation creep by climb and glide that are dominant at higher applied stress and diffusional creep that are dominant at lower applied stress. Finite element simulations are performed for the 3D cell model to investigate the creep response of Grade 91 and to understand the influence of various constitutive parameters.

The following points summarize the key developments related to the CP modeling framework and the key results of the simulations.

- The crystal plasticity material model platform in WARP3D developed prior to 2013 is extended to the multi-variable case by generalizing the framework of the constitutive equations and also the relevant subroutines in the code. The FORTRAN package for nonlinear equation solving, “nleqslv” [29] is incorporated into the material subroutine, providing both Newton and Broyden Secant method nonlinear equation solvers with line search and trust region modules. Also, the package provides features such as finite difference calculation of the Jacobian matrix and a checking script for validating the user-defined Jacobian. These enhancements add robustness to the nonlinear equation solver and also streamline the implementation of new constitutive models. A bookkeeping system of indices was created in order to reference the various quantities in the history vector and to simplify the output of state variables to text files in order to handle increasing complex constitu-

tive models. With these changes, the crystal plasticity model in WARP3D now represents nearly 27,000 lines of code in comparison to less than 4,000 lines in 2013 prior to commencing the efforts described in this report.

- A multi-variable dislocation density-based model was proposed for the body-centered cubic (BCC) systems of martensitic steel. The flow rule captures two key features of the material mechanisms. First, the lattice resistance or Peierls stress is considered to be the most significant short-range obstacle to dislocation motion. Second, during creep at high temperatures under sustained lower stresses, the motion of dislocations may be described through a glide-climb mechanism. The material parameters in the crystal plasticity model are calibrated against the experimental tensile data from Swindeman [45] for Grade 91. Subsequently, the creep response was investigated through the 3D cell model for two extreme cases: (a) grain boundary sliding and cavity growth suppressed by removing the interface elements in the mesh, and (b) sliding and opening mechanisms active along grain boundaries. Three creep simulations were conducted at the applied stress levels of 100 MPa, 120 MPa, and 140 MPa each at 600°C. For the case with active sliding and cavity growth, the simulated creep curve for 120 MPa load is rather close to the experimental data, since the interface material parameters were calibrated at 120 MPa. However, the response for other load levels is less accurate, and all simulated creep curves appear flatter than the corresponding measured curves, meaning that less evolution of the microstructure is captured in the model during early creep life. This discrepancy suggested that a different creep deformation mechanism is active at the lower stress levels that is not captured in the first proposed model.
- In pursuit of understanding the deformation mechanism transition in Grade 91 at lower operating stresses at temperatures at or below 600°C, a multi-mechanism crystal plasticity model is proposed that is a combination of dislocation creep and diffusional creep. To represent dislocation creep according to the climb plus glide mechanism, a power-law expression is adopted for the slip rate on the 12 primary BCC slip systems. The diffusional creep mechanism that is dominant at lower applied stress is represented through a linear viscous relation in terms of the deviatoric part of the stress tensor and a generic diffusion coefficient expressed by an Arrhenius relation. The power-law exponent and reference strain rate in the dislocation creep model were estimated by fitting the response of a single finite element model under constant imposed strain rate to the minimum creep strain rate test results for Grade 91 recorded in [23]. The diffusional creep coefficient was estimated by least-squares fit of the linear viscous diffusional creep relation to the measured minimum strain rates at lower applied stresses given by Kloc et al. [27].
- Creep simulations were conducted for the 3D cell model with the multi-mechanism crystal plasticity model combined with grain boundary sliding. The grain boundary sliding viscosity and normal direction stiffness were selected based on studies in Chapter 2 and Section 6.2, and then the crystal plasticity model parameters were such that the cell model

produced creep response in close agreement with the transient portion of the creep curves in [23]. For all of the load levels 100 to 160 MPa, the maximum discrepancy in the transient strain rate is a factor of two, and the simulated and experimental creep curves overlap for much of the strain history prior to onset of tertiary creep.

- The influence of the spatial arrangement of grain lattice orientations on the cell average creep strain rate and the local distribution of stress was investigated by considering five different spatial arrangements of the crystal lattice orientations in the grains of the cell model. These orientations are sampled from a random texture. For the applied load of 120 MPa at the elapsed time $t = 10^4$ hr, the maximum strain rate across the 5 simulations is $8.39 \times 10^{-7} \text{ hr}^{-1}$, the minimum rate is $7.51 \times 10^{-7} \text{ hr}^{-1}$, and the average is $8.01 \times 10^{-7} \text{ hr}^{-1}$, indicating that the difference is about 5%. The distribution of Mises stress over all finite elements in the cell model for the two spatial arrangements have similar tails but slightly different intermediate ranges. Thus, the distribution of orientations for random texture had a very mild effect on the bulk cell average creep rate during the primary and secondary creep regimes. Changes to the grain and grain boundary geometry may induce a larger change to the cell response, such as the results for periodic microstructures presented in Chapter 5.
- Several parameter studies were conducted on the 3D cell model to understand the effect of each of the main crystal plasticity constitutive parameters on the bulk deformation of the cell: initial flow stress τ_y , saturation stress τ_v , flow curve modulus θ_0 , and rate-sensitivity exponent n . The flow modulus θ_0 had a larger effect on the time to onset of tertiary creep compared with τ_v . Also, the parameter $\tau_y + \tau_v$ specifies the steady state creep rate reached by the model. Also, the creep behavior of the cell model was compared when the diffusional creep term was active and inactive within the grains. Creep strain rate curves at the higher stresses 140 and 160 MPa are nearly identical on the logarithmic scale whether or not diffusional creep is included. The larger minimum strain rates are most evident for the lower stresses of 100 and 110 MPa. The response of the cell model at the 100 MPa load level with and without the diffusional term are identical up to about 100 hours. The minimum strain rates with and without diffusional creep are $6 \times 10^{-7} \text{ hr}^{-1}$ and $2 \times 10^{-7} \text{ hr}^{-1}$ respectively, so that the diffusional mechanism accounts for about twice the flow compared to the crystallographic dislocation glide mechanism. Examination of fringe plots for Mises stress at lower applied stresses (10 MPa and 60 MPa) indicate that larger stress concentrations (factor of 4) occur at lower load levels on the cell model compared to higher load levels (factor of 2). Larger stress concentrations are likely accommodated in the grains when the linear viscous diffusional creep term is dominant compared to the power-law exponent of 12 in the dislocation creep regime. In the actual Grade 91 material, the local stress and strain state near a cavity population on a grain boundary is what is expected to drive the cavity evolution. Therefore, capturing the heterogeneity of these

fields is one benefit that the cell model provides over reduced order models that smear out the heterogeneities.

3.6 Chapter figures

Figure 3-2. Representation of 3D cell model for CP model creep simulations: fringe plot of first Kocks Euler angle to indicate orientation of crystal lattice.

Figure 3-3. Macroscopic cell strain rate (1/h) versus model time (h) for cell model without grain boundaries as a function of remote applied stress. (a) early portion of the creep response; (b) later portion of the creep response.

Figure 3-4. Macroscopic cell strain rate (/h) versus model time (h) for cell model with cavity growth and with sliding on grain boundaries as a function of remote applied stress.

Figure 3-5. Macroscopic cell strain rate (/h) versus model time (h) produced by the crystal plasticity model within the grains.

Figure 3-6. Variation of minimum creep strain rate with respect to applied stress from creep tests for Grade 91 at 600 C from Kimura et al. and Kloc et al. exhibiting mechanism regimes

Figure 3-7. Variation of minimum creep strain rate at lower stress levels from calibration of dislocation creep parameters against experimental data from Kimura et al. at 600 C

Figure 3-8. Variation of minimum creep strain rate at lower stress levels from calibration of diffusion coefficient against experimental data from Kloc et al. at several temperatures

Figure 3-9. Macroscopic cell strain rate (/h) versus model time (h) for cell model using calibrated material parameters including dislocation creep and diffusional creep within the grains and sliding along grain boundaries, compared to experimental data from Kimura et al.

Figure 3-10. Macroscopic cell strain rate (/h) versus model time (h), comparison of response for softening behavior in the dislocation creep model with cavity growth along grain boundaries at load level 100 MPa; the legend indicates the saturation stress τ_v as “Tv” and the flow modulus θ_0 as “Qo”

Figure 3-11. Macroscopic cell strain rate (/h) versus model time (h), comparison of response for different initial flow resistance and constant total saturation resistance at load level 140 MPa

Figure 3-12. Macroscopic cell strain rate (/h) versus model time (h), comparison of response for different values of flow modulus θ_0 at load level 140 MPa

Figure 3-13. Macroscopic cell strain rate (/h) versus model time (h), creep response from cell model with five different spatial arrangements (shuffling) of crystal orientations at load level 120 MPa

Figure 3-14. Frequency distribution of Mises stress field within grain finite elements of the cell model at applied load level 120 MPa: (a) first orientation arrangement; (b) second orientation arrangement

Figure 3-15. Macroscopic cell strain rate (/h) versus model time (h) for cell model using material parameters excluding diffusional creep, compared to experimental data from Kimura et al.

Figure 3-16. Macroscopic cell strain rate (/h) versus model time (h) for cell model using material parameters including diffusional creep, compared to experimental data from Kimura et al.

Figure 3-17. Macroscopic cell strain rate (/h) versus model time (h), creep response from cell model with and without the diffusional creep component at load level 100 MPa

Figure 3-18. Variation of minimum creep strain rate with respect to applied stress from cell model with and without the diffusional creep component in comparison to experimentally obtained rates for Grade 91 tests at 600 C from Kimura et al.

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4 Study of Numerical Issues from Grain Boundary Interfacial Stiffness

Several challenges were encountered during the numerical modeling of the microstructural response of Grade 91, most often manifesting as divergence of the Newton-Raphson equation solver at the domain level or material integration level. One of the most significant problems involved the quality of the interfacial traction fields obtained during preliminary studies. As described in Section 2.2.1.3, the normal component of the traction computed by the interface elements could exhibit oscillatory behavior with an order of magnitude greater than the applied stress level, particularly during the loading period and beginning portion of primary creep. This behavior is very detrimental to the accurate determination of the onset of cavity nucleation and growth by the cell model.

Therefore, an investigation was conducted to determine the relative effect of key model features on the appearance of oscillations in the traction field components: ratio of normal to tangential interface stiffness, polynomial order of finite element functions, and numerical formulation of impenetrability constraint.

4.1 Interface traction model description

Relatively few numerical studies have been performed using finite element modeling of representative volume elements containing crystal plasticity with the grains and interface elements along grain boundaries. Most such studies have focused on brittle fracture or crack propagation rather than on ductile void growth [56] [57] [58]. Earlier studies on two-dimensional microstructures considering elasticity [59] and power-law creep [60] revealed that heightened stresses can occur at triple junctions between grains when low sliding resistance is assumed within the models. Also, a wide body of literature exists on finite element contact mechanics modeling and the large stress concentrations that emerge when resolving normal and tangential contact tractions. Thus, a detailed study of the microstructural cell model's behavior under simplified interface constitutive models seemed justified to understand the phenomena reported in Section 2.2.1.3 regarding oscillatory numerical traction fields.

The 100 grain cell model is again considered as the testbed geometry. To focus on the interface behavior, linear isotropic elastic properties were assigned to all grain with $E = 150$ GPa and $\nu = 0.285$. Symmetry boundary conditions were applied on the planes intersecting $(0,0,0)$, and a uniform displacement $u_x = 0.001$ mm is applied on the $x = 0.2$ mm face such that the average uniaxial stress is approximately 750 MPa. The MATLAB finite element code mentioned in Section 3.2.1 was used for all simulations in this section in order to have a common platform and eliminate other sources of discrepancy.

Four different element types are compared: quadratic tetrahedral, linear tetrahedral, B-bar patch tetrahedral, and linear hexahedral. The B-bar patch formulation for tetrahedral elements involves an averaging of the volumetric strain over a patch of linear elements in order to remove volumetric locking [61] [62]. This element type, consisting of 8 linear elements grouped into a macro element with identical node structure or connectivity as a single quadratic tetrahedral element, was being considered as an option for WARP3D in order to combine linear polynomial interface elements with locking-free volumetric elements. A linear elastic version of the formula-

tion from [61] was implemented into the MATLAB code for this study. The finite element mesh for the tetrahedral meshes are topologically identical and have the same number of nodes. The hexahedral mesh is obtained by subdividing each quadratic tetrahedral element into four linear hexahedral elements, which introduces a new node for each element face in the model. Otherwise, all meshes have very similar numbers of nodes and degrees of freedom.

Two interface element formulations were compared. The first formulation is termed as “interface penalty method” and uses a linear relationship between the traction field $\mathbf{T}$ and the displacement gap field $\llbracket \mathbf{u} \rrbracket$ along the interface with different penalty or stiffness coefficients for the normal and tangential directions, referred to as K_n and K_t respectively. The tangential stiffness is meant to approximate the sliding behavior which is time dependent (viscous) for the microstructure simulations. Equal penalty values for tension and compression were employed, using just K_n , and thus the model is linear. The second formulation uses the same tangential penalty function coupled with a Discontinuous Galerkin (DG) treatment of the normal traction component [63] [64] [65]. The DG method is variationally consistent, meaning that the numerical solution converges toward a solution with zero penetration or gap without requiring an extremely large penalty parameter. The traction field is evaluated from a numerical fluxes as the weighted average of tractions from the continuum stress field along the interface: $T_n = \{\mathbf{n} \cdot \boldsymbol{\sigma} \cdot \mathbf{n}\} + \alpha_n \llbracket \mathbf{u} \cdot \mathbf{n} \rrbracket$ with $\{\mathbf{n} \cdot \boldsymbol{\sigma} \cdot \mathbf{n}\} = \mathbf{n}^+ \cdot [\delta^+ \boldsymbol{\sigma}^+ + \delta^- \boldsymbol{\sigma}^-] \cdot \mathbf{n}^+$ and the weights summing to unity. Details for calculating the weights and the penalty parameter as a function of element shape and size are given in [63].

4.2 Model response for low tangential stiffness

Most of the preliminary creep studies for Grade 91 in this project considered either free sliding (low viscosity) or no sliding (high viscosity). Therefore, the first testbed models with linear interface stiffness considered low tangential stiffness $K_t = 1.0$ MPa/mm. The normal direction penalty parameter was set much larger, as $K_n = 1.0 \times 10^6$ or $K_n = 1.0 \times 10^8$ MPa/mm. Figure 4-1 presents the axial displacement field u_x for the quadratic tetrahedral element mesh. Discontinuities in the field are clearly presented along grain boundaries, both for boundaries parallel to the load as well as perpendicular. The noticeable jumps on the perpendicular faces could be an indicator that (1) the normal stiffness is too low and elastic interface gaps are opening up or (2) some grain boundary elastic “sliding” has occurred such that two points adjacent in the current configuration are not adjacent in the reference configuration.

Next, the variations in the elemental stress field are compared for different formulations with different values of K_n . Figure 4-2 examines the stress field for the quadratic element mesh with $K_n = 1.0 \times 10^6$. Note that the element-average field is plotted, so that each triangle with a different color represents the face of a single finite element. The extreme values on the legend are set to the maximum and minimum stresses computed for this particular solution. The volume average stress field appears to be lower than the 750 MPa uniaxial tension value (150 GPa modulus times 0.5% strain). Figure 4-3 presents the stress field for the higher value $K_n = 1.0 \times 10^8$ with the same element type. A larger variation of stresses is evident, with some concentrations at boundaries and triple points. By comparison, the lower stiffness seems to reduce the stress concentrations by relaxing the enforcement of displacement continuity on the boundaries. The largest stresses appear within the smallest grains with closely spaced grain boundaries. Figure 4-4 presents similar re-

sults for the Discontinuous Galerkin method with quadratic elements for the stress field, suggesting that the behavior of this formulation is similar to the interface penalty method for the case of $K_n = 1.0 \times 10^8$. Linear polynomial elements display similar features of the stress field in Figure 4-5. Since there are 8 times more elements, more faces appear in the fringe plot, and the transition of color values is spatially smoother across the model. Figure 4-6 indicates that the hexahedral finite elements produce similar results to the tetrahedral elements. Finally, the legend in Figure 4-7 has been reset to the extreme values computed for the linear tetrahedral mesh with $K_n = 1.0 \times 10^8$; the stress concentrations are more easily seen to occur at triple points. In general, the continuum stress field is well behaved and does not have large oscillations.

The behavior of the interface traction field have much larger variations. The normal component of the traction field is presented in Figure 4-8 for the interface penalty method with stiffness $K_n = 1.0 \times 10^6$ on the quadratic finite element mesh. The traction values are all within the same magnitude as the average applied stress, and in general each planar grain boundary has a fairly uniform value of traction. Some faces are tensile while some are compressive. This behavior is not exhibited by the higher stiffness case in Figure 4-9 with the same formulation and finite element mesh. Now, neighboring elements on the same grain boundary have positive and negative traction values, meaning that oscillations are occurring between tension and compression with the magnitude of oscillations greater than the applied average stress. This result is obviously non-physical and would require mesh refinement to determine the true solution features. The situation does not improve for the Discontinuous Galerkin method in Figure 4-10 for the measure of the interface traction given by the combination of the traction average and the penalty term, called at the “total traction field”. The portion of this field from the average continuum traction field, shown in Figure 4-11, is somewhat more stable, which agrees with the stress contour fields in Figure 4-4. However, the inelastic interface constitutive functions for the Discontinuous Galerkin method, such as debonding [64], are a function of the total traction field. Thus, the numerical formulation does not strongly affect the computed solution quality for the large value of normal stiffness K_n .

The solution fields for B-bar patch elements in Figure 4-12 and linear tetrahedral elements in Figure 4-13 also display very large oscillations. The fields appear slightly smoother compared to Figure 4-9, with less dark red faces adjacent to dark blue faces. This improved appearance may be due to the finer resolution of the plotted contour fields since the fields are displayed for individual elements. Lastly, the oscillations are also present for linear hexahedral elements in Figure 4-14. Thus, changing the element type also does not improve the quality of the interface traction field, meaning that the poor performance cannot be attributed solely to the features of quadratic interface elements. Rather, the solution for this linear elastic model, which can be mathematically proven to possess a unique solution, can only be determined through mesh refinement.

While the behavior of the interface traction is a primary concern for stability of the cavity growth model, the elastic separation of the interface must also be controlled so that the microstructural model is not artificially compliant. The computed normal displacement gap for the case with $K_n = 1.0 \times 10^6$ shown in Figure 4-15 is therefore concerning. The extreme values of the gap, shown by the legend, are about 40-50% of the applied displacement field, while the intermediate values are about 1% of the applied displacement. Also, the values are nearly uniform on each grain boundary. In fact, the color values on each interface element are identical between the traction field Figure 4-9 and gap field Figure 4-15, which is a consequence of the linear relationship

in the penalty constitutive equation. The large interface gaps highlight the importance of properly calibrating the penalty coefficient, a known issue with cohesive interface element formulations [12] [64]. Figure 4-16 examines the displacement gap for the interface penalty method on the quadratic element mesh with $K_n = 1.0 \times 10^8$. The gap magnitude has decreased by a factor of 10, but now oscillations are present across grain boundaries, likely due to the weak enforcement of impenetrability which balances the positive and negative errors. Similar trends are exhibited by the Discontinuous Galerkin method (Figure 4-17), linear tetrahedral elements (Figure 4-18), and linear hexahedral elements (Figure 4-19).

4.3 Model response for high tangential stiffness

Returning to the discontinuities of the displacement field in the continuum plot shown in Figure 4-1, these discontinuities seem to be larger than expected for a polycrystalline material that has a small number of voids and cracks. Rather, the behavior appears to more closely represent a closely-packed granular material with particles in contact along interfaces. Thus, while large amounts of grain boundary sliding might occur at much larger temperatures, most likely a larger value of interface tangential stiffness and viscosity are needed to more closely represent the microstructure response at the moderate temperatures being studied herein. Also, the frictionless contact of individual spheres considered by Hertzian contact, reviewed for example in [65], is known to produce sharp gradients in contact pressures that are only resolved on very fine grids and lead to oscillations on coarse grids without special numerical treatments.

All of these considerations suggested that a larger value of interface tangential stiffness should be employed. Figure 4-20 presents the normal traction field for linear tetrahedral elements using the interface penalty method with several different values of K_t , all with $K_n = 1.0 \times 10^8$. Notice that as the tangential stiffness is increased from part (a) to part (c), the oscillations in the normal direction on boundaries decrease. The results for Figure 4-20 (a) with $K_t = 1.0 \times 10^6$ have similar degrees of oscillation to the results in Figure 4-20 (d) with $K_t = 1.0$, which is a duplication of Figure 4-13 with a different legend. The smoothness of the boundary fields is acceptable for both Figure 4-20 (b) and (c) with the larger stiffness. The fringe plots of displacement gap in Figure 4-21 exhibit similar trends; studies for quadratic meshes also show similar trends. As mentioned above, the oscillations that appear for the lower values of stiffness may be due to sharp contact pressure developing similar to those for Hertzian contact. The finite element mesh with only 20 interface elements per grain boundary is not sufficiently refined to capture the concentrated pressure from pinching at triple points.

4.4 Interface penalty stiffness conclusions

The improvement to the interface normal tractions obtained in Section 5.3 by increasing the value of K_t suggest that a reasonable range for the tangential stiffness to avoid artificial oscillations in the normal traction on coarse meshes is a value that is within a factor of 10 to 100 of the normal direction stiffness. This range of values is appropriate for each of the studied numerical formulations and element types. To translate this recommendation back to the nonlinear constitutive models for cavity growth described in Section 2, relevant estimates of physically realistic values for grain boundary sliding viscosity are needed. From a review of literature conducted in [12] [66] and references therein, reasonable values for the grain boundary diffusivity of Grade 91 at the temperature of 600 C are on the order of 10^{-16} to 10^{-14} $\text{MPa}^{-1} \cdot \text{hr}^{-1} \cdot \text{mm}^3$. Assuming an in-

verse relation of the viscosity to diffusivity, moduli additional physical constants, corresponding values of viscosity lie between 10^5 to 10^7 $\text{MPa} \cdot \text{hr} \cdot \text{mm}^{-1}$. Therefore, an intermediate value of $\eta_b = 10^6$ is adopted for the numerical studies in Section 6, in light of the effect of grain boundary sliding on primary creep determined in Section 6.3. Thus, a related estimate for the normal stiffness $K_{lin}^{user} = 1.0 \times 10^8$ is considered for these simulations as well, and was found to provide stable computed field for the interface normal traction.

4.5 Chapter figures

Figure 4-2. Stress field σ_{xx} for interface penalty method with $K_n = 1 \times 10^6$ and $K_t = 1 \times 10^0$, quadratic tetrahedral elements.

Figure 4-3. Stress field σ_{xx} for interface penalty method with $K_n = 1 \times 10^8$ and $K_t = 1 \times 10^0$, quadratic tetrahedral elements.

Figure 4-4. Stress field σ_{xx} for Discontinuous Galerkin method with $K_n = 1 \times 10^8$ and $K_t = 1 \times 10^0$, quadratic tetrahedral elements.

Figure 4-5. Stress field σ_{xx} for interface penalty method with $K_n = 1 \times 10^8$ and $K_t = 1 \times 10^0$, linear tetrahedral elements.

Figure 4-6. Stress field σ_{xx} for interface penalty method with $K_n = 1 \times 10^8$ and $K_t = 1 \times 10^0$, linear hexahedral elements.

Figure 4-7. Stress field σ_{xx} for interface penalty method with $K_n = 1 \times 10^8$ and $K_t = 1 \times 10^0$, linear tetrahedral elements. Maximum and minimum of legend correspond to $K_n = 1 \times 10^8$ results.

Figure 4-8. Normal traction component field $T_n = K_n \llbracket \mathbf{u} \cdot \mathbf{n} \rrbracket$ for interface penalty method with $K_n = 1 \times 10^6$ and $K_t = 1 \times 10^0$, quadratic tetrahedral elements.

Figure 4-9. Normal traction component field $T_n = K_n \llbracket \mathbf{u} \cdot \mathbf{n} \rrbracket$ for interface penalty method with $K_n = 1 \times 10^8$ and $K_t = 1 \times 10^0$, quadratic tetrahedral elements.

Figure 4-10. Normal total traction field $T_n = \{n \cdot \sigma \cdot n\} + K_n \llbracket u \cdot n \rrbracket$ for Discontinuous Galerkin method with $K_n = 1 \times 10^8$ and $K_t = 1 \times 10^0$, quadratic tetrahedral elements.

Figure 4-11. Normal flux traction field $T_n = \{n \cdot \sigma \cdot n\}$ for Discontinuous Galerkin method with $K_n = 1 \times 10^8$ and $K_t = 1 \times 10^0$, quadratic tetrahedral elements.

Figure 4-12. Normal traction component field $T_n = K_n [u \cdot n]$ for interface penalty method with $K_n = 1 \times 10^8$ and $K_t = 1 \times 10^0$, B-bar patch elements.

Figure 4-13. Normal traction component field $T_n = K_n [u \cdot n]$ for interface penalty method with $K_n = 1 \times 10^8$ and $K_t = 1 \times 10^0$, linear tetrahedral elements.

Figure 4-14. Normal traction component field $T_n = K_n [[u \cdot n]]$ for interface penalty method with $K_n = 1 \times 10^8$ and $K_t = 1 \times 10^0$, linear hexahedral elements.

Figure 4-15. Normal displacement gap field $[[u \cdot n]]$ for interface penalty method with $K_n = 1 \times 10^6$ and $K_t = 1 \times 10^0$, quadratic tetrahedral elements.

Figure 4-16. Normal displacement gap field $\llbracket u \cdot n \rrbracket$ for interface penalty method with $K_n = 1 \times 10^8$ and $K_t = 1 \times 10^0$, quadratic tetrahedral elements.

Figure 4-17. Normal displacement gap field $\llbracket u \cdot n \rrbracket$ for Discontinuous Galerkin method with $K_n = 1 \times 10^8$ and $K_t = 1 \times 10^0$, quadratic tetrahedral elements.

Figure 4-18. Normal displacement gap field $\llbracket u \cdot n \rrbracket$ for Discontinuous Galerkin method with $K_n = 1 \times 10^8$ and $K_t = 1 \times 10^0$, linear hexahedral elements.

Figure 4-19. Normal displacement gap field $\llbracket u \cdot n \rrbracket$ for Discontinuous Galerkin method with $K_n = 1 \times 10^8$ and $K_t = 1 \times 10^0$, quadratic tetrahedral elements.

5 True Periodic Boundary Conditions

5.1 Background

The goal of the simulations described in this report is to represent a statistically representative volume element (RVE) and use the response of the RVE to represent the response of the material on the macroscale. When deciding on an appropriate RVE the first task is to ensure that it is statistically representative of the overall material structure and sufficiently large to capture the full distribution of microstructural features and deformation modes important in the actual material [67] [68] [69]. Previous reports have established that the cell used here is adequately representative in this sense.

Once the structure and size of the RVE is established, for example the grain size and shape distribution, the material texture, the distribution of grain and GB material properties, and the number of grains modeled in the cell, it must be discretized and boundary conditions established to impose macroscale loading conditions. This work uses the open source software Neper [70] to create the discretization. At least two possibilities exist for the RVE shape and applied boundary conditions: a “block” model of the type shown in Figure 5-1a and a true-periodic model shown in Figure 5-1b. Both RVEs instantiate the same material properties, i.e. the same texture, grain size distribution, etc. The block RVE truncates the statistically-representative structure into a cube, whereas the true periodic structure contains only whole grains. Both structures tile space. For the block RVE this is trivial – a tessellation of cubes fills space with gaps or overlaps. For the periodic structure this requires special consideration to ensure that the structure tiles correctly. Figure 5-2 shows that Neper generates periodic RVEs that fill space. Neper does this by creating a periodic Voronoi tessellation [21].

For both RVEs the mesh is periodic – the nodes and element faces match in the tiled structure. This allows imposing the correct boundary conditions (BCs) using multi point constraints (MPCs) in the finite element solver. Additionally, the true-periodic RVE requires cohesive elements inserted not only on the interior grain boundaries fully inside the cell but also on the outside faces of the grains to allow sliding and opening on the periodic interfaces. Inserting these cohesive elements requires a sophisticated algorithm, described in Chapter 5.

The objective of a set of BCs for a RVE is to ensure that 1) the structure remains periodic under subsequent deformation and 2) to allow the user to impose the macroscale loading conditions of interest. The details of the block RVE boundary conditions have been described in previous reports. Essentially, MPCs are used to ensure that opposite faces of the cube remain plane and parallel. Then either a force or a displacement is applied to one or more faces of the model. These forces or displacements impose uniform stresses or strains in the directions of the cube faces. It is much more difficult to impose more complicated loading conditions on the block RVEs.

The boundary conditions for the periodic RVE are more complicated and described in detail below. These boundary conditions can directly impose arbitrary macroscopic deformation gradient and/or stress tensor components on the periodic cell. Therefore, the periodic model can easily represent arbitrary macroscale boundary conditions.

Each type of RVE has advantages and disadvantages. For the block RVE:

- the model is relatively simple to create, not requiring periodicity when creating the model geometry;
- loading conditions in the direction of the cube faces are easy to impose and the required MPCs are easy to generate;

but:

- loading conditions not in the directions of the cube faces/edges are difficult to impose;
- this structure cuts grains arbitrarily and effectively creates artificial grain boundaries across the periodic faces on these cuts.

Whereas for the periodic RVE:

- arbitrary macroscale loading conditions are easily imposed;
- the model is a direct instantiation of a representative microstructure, without any artificial cuts;

but:

- the model geometry can be difficult to create;
- meshing the periodic geometry can be difficult, possibly resulting in a poor quality mesh
- the MPCs imposing periodic deformation are more difficult to set up.

The key question for the material deformation modeled here – creep deformation to rupture, with creep damage represented with cohesive elements on the grain boundaries – is whether the artificial boundaries created by cutting the structure into a cube affect the quality of the results. The artificial boundaries formed in this process are not representative of the actual material GB distribution and may cause artificial stress concentrations. More importantly, the interior grain boundaries terminating on the cube surface are artificially locked against sliding – they are forced to slide into a solid grain on the other side of the periodic interface. Both of these effects could potentially degrade the accuracy of a block-type model, potentially requiring a larger RVE size to minimize the influence of the artificial surfaces by increasing the volume to surface area ratio. This chapter answers this question by implementing true periodic boundary conditions in WARP3D and comparing block RVEs to corresponding true periodic structures.

5.2 Implementation

5.2.1 Solid and interface finite elements

Simulation of grain and grain boundary deformation with the models described in Chapters 2 and 3 requires grains defined by solid elements and boundaries defined by 3D interface elements. Neper generates the solid mesh directly, including appropriate periodicity. A MATLAB program [71] inserts the interface elements along grain and packet boundaries.

Neper can generate 3D meshes with both first order and second order tetrahedral elements. The two available tetrahedral elements in WARP3D are *tet4* and *tet10*. The *tet10* element provides a quadratic displacement field and better represents bending deformations without severe shear locking. Under fully incompressible plastic deformations *tet10* exhibits minimal volumetric locking, even when the element edges are curved. Therefore, this report uses *tet10* elements to represent the grain bulk.

WARP3D has 12-node triangular-shaped (*trint12*) interface elements that provide displacement compatibility with faces of the *tet10* solid elements. The *trint12* elements may be non-planar and may have curved edges in both the initial and deformed configurations. These initially zero-thickness elements have top and bottom surfaces coupled with a cohesive constitutive model that links three displacement jumps across the surfaces to three work-conjugate tractions. The interface elements are programmatically separate from the traction-displacement cohesive material models; new cohesive models can be incorporated without reimplementing the element routines.

5.2.2 Interface element insertion

Neper currently cannot generate interface elements for quadratic solid elements. Therefore, this report uses Neper only to generate the solid mesh and the element sets describing each grain. A separate preprocessor inserts interface elements between the solid elements on grain boundaries. The interface-insertion preprocessor wraps an algorithm and MATLAB code developed by Truster [71]. The self-contained algorithm requires only nodal coordinates, element connectivity, and element sets for each grain. The interface insertion algorithm duplicates nodes and creates zero-thickness interface elements that conform to the topology and order (linear or quadratic) of the attached solid element faces.

A Python script reads the Neper output and translates it to the format required by the MATLAB interface-insertion script. Briefly, to insert cohesive elements in a *non-periodic* do-

main the script: (1) finds and catalogs all facets shared by elements in the mesh; (2) duplicates the nodes along facets that coincide with grain boundaries; (3) updates the connectivity of adjacent solid elements; and (4) generates the connectivity of the interface elements.

Generating cohesive elements for periodic domains required modification of the existing non-periodic interface insertion algorithm. In addition to the information required for non-periodic domains the periodic domain insertion script requires a list of node pairs on opposite sides of the domain corresponding to the multi-point conditions, as described in Section 5.2.3. Using these pairs, the modified script first collapses the connectivity of the so that only one node remains from each pair or group of node pairs. This directly connects periodic boundaries, turning the RVE mesh into a toroid. The existing routines can then insert cohesive elements on the grain boundaries, now including the toroidal periodic boundaries. Finally, the modified method splits the toroidal mesh by duplicating nodes and generates the appropriate MPCs to enforce periodic boundary conditions. The script ensures that all interface elements of a particular grain boundary are inserted on the same side of the domain

5.2.3 Periodic boundary conditions theory

Consider a 3D, periodic structure with lattice vectors $\mathbf{a}_i$ for $i = 1, 2, 3$. Let the displacement field in the periodic structure be $\mathbf{u}$, the deformation gradient be $\mathbf{F}$, and the 1st Piola-Kirchhoff stress tensor be $\mathbf{P}$. Consider two points $\mathbf{p}_1$ and $\mathbf{p}_2$ such that

$$\mathbf{p}_1 = \mathbf{p}_2 + \sum_{i=1}^3 n_i \mathbf{a}_i = \mathbf{p}_2 + \mathbf{a}_{12} \quad (5.1)$$

for some integers n_i . Let the corresponding displacements of these two points be $\mathbf{u}_1$ and $\mathbf{u}_2$. In the undeformed state these two points are equivalent under the lattice symmetry. To maintain the lattice symmetry they must remain equivalent under subsequent deformation. Therefore,

$$\mathbf{p}_1 + \mathbf{u}_1 = \mathbf{p}_2 + \mathbf{u}_2 + \mathbf{a}'_{12} \quad (5.2)$$

where $\mathbf{a}'_{12}$ is the lattice vector in the deformed configuration, given by

$$\mathbf{a}'_{12} = \mathbf{F} \cdot \mathbf{a}_{12} \quad (5.3)$$

Combining Equations (5.2) and (5.3) yields

$$\mathbf{u}_1 = \mathbf{u}_2 + \mathbf{a}'_{12} - \mathbf{a}_{12} = \mathbf{u}_2 + (\mathbf{F} - \mathbf{I}) \cdot \mathbf{a}_{12} \quad (5.4)$$

or

$$\mathbf{u}_1 - \mathbf{u}_2 = (\mathbf{F} - \mathbf{I}) \cdot \mathbf{a}_{12} \quad (5.5)$$

Equation (5.5) is an inhomogeneous constraint equation. With a periodic mesh these constraints can be imposed as MPCs tying equivalent nodes in the periodic RVE, i.e. nodes with images translated across the structure by some integer combination of lattice vectors. One such con-

straint is required for each node pair and each node may belong to multiple pairs. Each vector constraint equation represents three scalar constraints.

Danielsson, Parks, and Boyce [72] suggest implementing these equations by using dummy degrees of freedom (DoF) describing the nine components of the deformation gradient. For example, three free-floating nodes might be used with each of their nine deformation degrees of freedom representing one component of the deformation gradient. This transforms the system into a series of MPCs involving three deformation degrees of freedom – two from the periodic nodes and one from the dummy degree of freedom – and constraints on each of the dummy degrees of freedom. DPB show through virtual work that the nodal forces corresponding to the dummy degrees of freedom correspond to the volume of the unit cell times the macroscopic first Piola-Kirchhoff stress tensor, i.e. the nine components of the tensor $\mathbf{I}\mathbf{P}$. Applying the periodic MPCs results in 9 unconstrained degrees of freedom: the dummy DoF. Adding a displacement constraint to one of these dummy DoF imposes a component of the macroscale deformation gradient on the RVE. Applying a force imposes a component of the macroscale stress tensor. This configuration allows the user to easily impose arbitrary macroscale boundary conditions.

Given a periodic mesh of a periodic geometry and a list of lattice-equivalent boundary node pairs and their corresponding lattice vectors conceptually the procedure for imposing the periodic boundary conditions is straightforward: for each periodic node impose the three scalar constraint equations given by Equation (5.5). The required information – the periodic mesh and list of equivalent node pairs – is an output of Neper and the pre-processing script described in this report for inserting periodic cohesive elements on the outside faces of a periodic model.

One complication is this procedure does not remove rigid body modes. The three translational modes can be removed by constraining all displacements of an arbitrary node in the interior of the mesh. The three rotations can be removed by finding three additional interior nodes and constraining one displacement degree of freedom on each, one x-displacement, one y-displacement, and one z-displacement. Alternatively, the rigid modes can be eliminated by removing 9 scalar MPCs and replacing them with displacement constraints.

5.2.4 *Implementing periodic boundary conditions in WARP3D*

Unfortunately, this strategy cannot be used directly to apply periodic boundary conditions in WARP3D. The MPCs described above are inhomogeneous. Actually, the MPCs directly setup by the DPB method are homogeneous but one DoF in each set is constrained, therefore leading to an inhomogeneous MPC of the type described by Equation (5.5) after substitution. WARP3D does not have the ability to impose inhomogeneous multipoint constraints. There are at least three ways to implement MPCs in finite element solvers: 1) Lagrange multipliers augmenting the nonlinear equilibrium equations 2) directly condensing out the constrained equations, 3) augmenting the equilibrium equations with penalty equations approximately enforcing the constraints. WARP3D uses the second method which has the advantage of removing DoF from the overall system, instead of adding additional DoF, increasing the size of the system of equations. This method requires logic to rearrange the internal force side of the equilibrium equations to remove the appropriate equations. Inhomogeneous constraints would require similar logic to rearrange the external force equations, but this logic was never implemented in WARP3D.

An alternative to implementing inhomogeneous boundary conditions in the code is to enforce the periodic constraints as a series of homogeneous MPCs and then drive the dummy DoF in the

MPCs using a penalty term. While somewhat contrived this method has implementational advantages in WARP3D. The method is identical to that of DPB except instead of constraining the dummy DoF directly instead the dummy DoF constraints are imposed through a penalty term. In detail, WARP3D creates two sets of three dummy nodes for a total of 18 extra DoF. The procedure described above generates MPCs tying the equivalent node pairs to the first set of nine dummy DoFs. Then the first nine dummy DoFs are tied to the second nine dummy DoFs through nine penalty constraints. The loading conditions – deformation gradient or stress tensor components – are imposed through the second set of dummy DoFs. With an adequately high penalty stiffness this method produces identical results that of DPB.

This strategy required implementing penalty constraints in WARP3D. This was done by adding a new element type taking as input two nodes in the connectivity table. The three DoF of each node are then tied together by three penalty stiffnesses. This is nearly a linear spring element except the stiffness matrix is always diagonal so it does not account for the orientation of the spring. Instead it directly ties the corresponding nodal DoF together: x-displacement to x-displacement, y-displacement to y-displacement, and z-displacement to z-displacement.

After implementing the penalty elements a complete periodic test simulation was setup for an arbitrary periodic RVE generated in Neper. Each grain was given different linear elastic properties and no cohesive elements were used on the boundaries – they were treated as rigid. Then the complete system was tested by imposing different combinations of stress tensor components and displacement gradient components, running the linear simulation, and post-processing the results in Paraview [73] to ensure the simulations produce the correct average stresses and strains. Additionally, the penalty stiffness was adjusted to give good accuracy – the stress and displacement gradient components in the results match those imposed – without affecting the numerical performance of the model. For units of MPa and mm a penalty stiffness of 10^6 MPa/mm was found to be optimal.

5.3 Comparison between periodic and block RVEs

Two models were used to evaluate the differences between periodic and block RVEs. The first is a simplified model that compares two RVEs with identical grain geometries. The second is an instantiation of the full model described in this report. Both models use quadratic tetrahedral elements with a 4-point $\bar{B}$ integration scheme designed to prevent numerical issues caused by incompressible plastic deformation. The block geometries have cohesive elements inserted on the interior grain boundary faces and use the periodic boundary conditions described in previous reports. The periodic models have cohesive elements both on the interior and exterior grain faces, inserted using the algorithm described in Section 5.2.2, and periodic boundary conditions of the type described in this chapter. All comparisons are for creep loading: a dead-load stress (i.e. a component of the first Piola-Kirchhoff stress tensor) prescribed in one axial direction and zero stresses in all other directions.

5.3.1 Simplified model

Figure 5-3 shows the simplified model used to examine differences between the two RVE types. This model contains 100 grains and the block and periodic geometries are identical – they both have the same grain structure. However, the meshes produced for the two geometries are different. Table 5-1 describes the block and periodic mesh parameters.

Neper provides a geometry regularization option. This option removes small grains and small grain faces and generally produces a geometry from which a tetrahedral mesher can generate a high-quality finite element mesh. However, this option cannot be used with periodic geometries and without it the resulting meshes tend to be poor quality. For the full model – crystal plasticity and the cohesive-interface GB elements representing creep damage – this severely limits the amount of deformation that the model can develop before it breaks down numerically, generally by a convergence failure in the crystal plasticity routines. Usually, unregularized geometries fail before the onset of tertiary creep.

To avoid this issue while still retaining identical geometries for the block and periodic RVEs this comparison simplified the constitutive description of the grains and GBs. For the grains the models use crystal plasticity with random grain orientations but arbitrary Voce hardening parameters designed to ensure the grain bulk response continues to harden out to large strains. This avoids numerical instability in the grain bulk. For the GBs the simplified comparison models use linear viscous GB sliding but linear elastic GB opening, essentially turning off creep damage.

Figure 5-4 compares the creep strain accumulated over time in the block and periodic models. The figure shows the total creep strain as well as the strain accumulated in the loading direction due to GB sliding and bulk grain deformation. Because these are the only two mechanisms present in this simulation, the total of the two decomposed strains equals the total creep strain. The figure shows that there are some small differences between the results of the two models but no significant differences between the two approaches.

Figure 5-5 and Figure 5-6 clearly show the statistical similarity of the two models. Figure 5-5 is a histogram of the von Mises stress in each solid element in the two models at the last load step. Figure 5-6 is a similar histogram showing the grain boundary sliding rates in each cohesive element, also during the last load step. The grain bulk stress distributions are nearly identical. The GB sliding rates show larger differences but are still representative of the same statistical distribution. This figure strongly suggests that there is little difference between the simulation results for the two RVE approaches. In particular, Figure 5-6 suggests that the cut RVE faces and the corresponding terminated interior grain boundaries in the block RVE do not significantly affect grain boundary sliding. The block model artificially terminates the boundaries at the edge of the cubic cell. In the true periodic model these grain boundaries terminate into other realistic grain boundaries, forming triple points in 2D sections. Likely both termination conditions provide a similar level of constraint: both are very difficult to slide past.

5.3.2 *Full model*

The previous results are for a simplified description of the material response, designed to allow for the accumulation of significant creep strain before the simulation fails. The lack of a periodic regularization option in Neper necessitated this approach. This subsection compares simulation results from unregularized block and periodic RVEs. Here, the grain geometry parameters were tuned to produce an approximately regularized grain structure without explicit regularization to improve the grain geometry. However, this means that the block and periodic RVEs are not of identical grain structures. Instead, they are statistically equivalent – drawn from the same grain size, shape, and orientation distributions – and both use the same material properties and models – the full model described in previous chapters, including linear viscous grain bulk behavior designed to mimic diffusional mechanisms and the full grain boundary damage model.

Figure 5-1 shows the two RVEs used for the comparison. Both consist of approximately equal volume, highly spherical grains designed to be easy to mesh. The grain sizes and shapes are statistically identical, but the block (a) and periodic (b) models are different instantiations of the underlying statistical distributions. The material properties are those described in this report for the full final model of creep deformation in Grade 91.

Other results for block RVEs described in this report use the mesh regularization option to ensure Neper produces a high quality finite element mesh. Even though the grain properties used to generate the RVEs used here are designed to produce high quality meshes, the meshes are still not as regular as those produced with the regularization option. This means that several of the simulations do not enter the tertiary creep regime. However, this section compares the primary creep portion of the simulation response to see if there are any significant differences between the two simulation approaches. Table 5-2 describes the properties of the block and periodic meshes.

Figure 5-7 shows the creep rate versus time for 16 simulations: eight different load levels (60, 80, 100, 120, 140, 160, 180, and 200 MPa) and 2 different model types (block and periodic). For the higher load levels there is very little difference between the two model types – the creep curves are essentially identical. Differences in this regime are numerical; the periodic models tend to fail to converge before the block models. At the lower stress levels there is a significant difference between the block and periodic models in the initial, primary creep portion of the curve.

The remaining figures in this chapter (Figure 5-8 to Figure 5-13) plot the results of the two types of simulations, block and periodic, for three different load levels: 60, 140, and 200 MPa. These plots break down the average, macroscale strain rate in the model into several deformation mechanisms. At the highest level they plot the total deformation rate. On a second level they divide that total creep deformation rate into two categories: grain bulk and grain boundary. Finally, on a third level they divide the grain bulk rate into elastic, crystal plasticity, and linear viscous contributions and the grain boundary behavior into GB opening and sliding terms. The total of the contributions on each level equals the overall strain rate. Furthermore, two figures are shown for each load level. The first shows strain rates in the direction of the loading, these would be the measured creep strain rates. The second shows von Mises-type effective strain rates, including transverse and shear deformation components.

In general, the two types of strain rate data – loading and effective – show similar trends. One noticeable difference is in the elastic strain rates. The macroscale elastic strain rate in the loading direction can become compressive, representing macroscale softening. This causes it to jump off the log scale plot. The effective strain rate data is always positive and shows a smooth curve, however it is does not correspond to an easily experimentally measured quantity.

Figure 5-8 and Figure 5-9 elucidate the differences between the two RVE approaches at low stresses. In this regime the isotropic, diffusional grain deformation term dominates the crystallographic, crystal plasticity deformation. Additionally, the overall deformation rate is low, including the GB sliding rate. The two most important mechanisms in the primary creep regime in both models are the linear viscous grain bulk term, representing diffusional deformation mechanisms, and grain boundary sliding. Both models eventually reach a state of secondary creep at a constant rate where the deformation in both cells is nearly identical – even broken down into components. The differences between the two models are in the primary creep regime. Note that the higher

loading stress levels never undergo anything resembling a steady, secondary creep rate, instead transitioning directly from primary to tertiary creep.

The difference between the block and periodic RVEs is in how long it takes to reach secondary creep – the periodic structure takes longer to achieve a constant creep rate. This difference is due to GB sliding. The onset of steady, secondary creep is when GB sliding deformation becomes small, essentially because all the easy GB sliding has taken place and the grains are essentially trapped at triple points. At higher stresses this takes place relatively quickly but it takes longer at the lower stress level and longer in the periodic model, compared to the block model. Presumably, each grain has a certain distance of “free” GB sliding available to it before it meets a substantial obstacle like a triple point. At high stresses this free sliding occurs quickly because the stresses driving the viscous sliding are large. Therefore, any statistical differences in the free sliding path lengths between the periodic and block models are overwhelmed by the short time required for the grains cover these distances.

At the lowest stress level this process of exhausting free sliding takes longer due to the low driving force. This means any differences in the free sliding path lengths between the two models are accentuated. The periodic model has a longer period of free sliding, which might indicate that the “cut” surfaces in the block RVE do impeded GB sliding, as suggested. Note the results in the previous subsection on the simplified model were for a high loading stress. This implies that the periodic RVE might have a significant advantage over the block RVE for low stress, diffusion-driven creep deformation. However, this period of primary creep is exhausted relatively quickly even at low stress and the steady-state secondary creep rates and time-to-tertiary creep are essentially the same for the block and periodic models. So the difference may be significant only for very low loads or when it is important to accurately model primary creep.

Figure 5-10 and Figure 5-11 for 140 MPa and Figure 5-12 and Figure 5-13 for 200 MPa show similar behavior. Elastic grain bulk deformation dominates the loading portion of the simulation. Next comes a period of primary creep dominated by grain bulk plasticity and grain boundary sliding. When the model exhausts free GB sliding the GB opening rate increases, indicating the onset of damage and tertiary creep. The block and periodic models have very similar responses with no significant differences between the two modeling strategies.

Table 5-3 shows the time to the onset of tertiary creep for the block models for all the loading stresses considered here. For this table the time to tertiary creep is defined as the time when the total deformation rate in the loading direction increases to reach a value 20% greater than the minimum, total loading direction strain rate. All the block models except one achieve this condition, which might be considered a reasonable surrogate for total creep life. With the exception of the two lowest load levels none of the periodic models extend to tertiary creep, all failing prior to the start of tertiary creep because of convergence problems in the crystal plasticity model. Table 5-3 defines a time to grain boundary opening as the time at which the grain boundary opening rate, in the direction of loading, increases to above 10% of the minimum grain boundary opening strain rate, in the direction of loading. The table shows that this time roughly correlates with the time to tertiary for the block model and so could serve as another surrogate for creep life. All the periodic model simulations, except one, extend past this time which means it could be a useful measure of creep life for the periodic models. The time to opening in the periodic models roughly matches the time to opening for the block models, with the exception of the two lowest stress levels. Differences between the two types of models in this regime were described above.

5.4 Summary

Overall, this chapter shows only small differences in the simulation results when comparing the periodic and block RVE methodologies. This is in agreement with past results, including those of [74]. However, there are some differences between the two approaches in the primary creep regime and at low stresses, both areas where GB sliding is an important deformation mechanism. This chapter attributes these differences to artificial constraint on GB sliding caused by the sliced faces of the block RVEs. However, secondary and tertiary creep occur at roughly the same time and the same level of deformation in both the periodic and block models, suggesting that any difference is transitory and confined to the primary creep regime.

A clear advantage of the periodic RVE is the ease of applying different macroscale boundary conditions to the model. This will be used in a subsequent chapter to examine at the effect of tri-axiality on the model response to explore notch strengthening and weakening effects in Grade 91. Furthermore, this chapter establishes the time to GB opening as a reasonable surrogate for the time to the onset of tertiary creep. This surrogate is necessary when using results from periodic RVEs as they rarely achieve a significant amount of tertiary creep before failing to converge.

5.5 Chapter figures

Figure 5-2. The true periodic RVE tiles space. This figure shows a 2x2x2 tiling of the RVE cells. Both the mesh and geometry are periodic.

a)

b)

Figure 5-3. Simplified model for directly comparing block and periodic geometries. Note the grain structure in the block (a) and periodic (b) RVEs are identical. However, due to the requirement of mesh periodicity, the tetrahedral meshes are not the same.

Figure 5-4. Strain rate comparison between the simplified block and periodic RVEs. The solid lines show results for the block RVE and the dashed lines for the periodic RVE. The figure compares the total strain rates, the grain bulk strain rates, and the grain boundary sliding strain rates.

Figure 5-5. Histogram comparing the distribution of the element von Mises stresses generated in the simplified block RVE and the simplified periodic RVE.

Figure 5-6. Histogram comparing the distribution of the element GB sliding rates generated in the simplified block RVE and the simplified periodic RVE.

Figure 5-7. Plot showing the effect of the two different RVEs for the full model at various stress levels. The data series are the total strain rate in the opening direction for each model.

Figure 5-13. Plot comparing effective strain rates for the block and periodic RVEs for a load of 200 MPa.

Table 5-1. Description of identical-grain block and periodic meshes used to evaluate the effects of periodic boundary conditions on the simplified model.

Model	Number of nodes	Number of elements	Number of cohesive elements
Block	54829	32964	7984
Periodic	88282	48578	12116

Table 5-2. Description of the statistically-equivalent block and periodic models used to evaluate the effects of periodic boundary conditions on the full simulation framework.

Model	Number of nodes	Number of elements	Number of cohesive elements
Block	29452	16869	4452
Periodic	39086	19797	6053

Table 5-3. Time to minimum GB opening rate for several stress levels comparing the periodic and block simulations. The table includes a column for time to the start of tertiary creep, which could only be reliably computed for the block models. A > symbol in the time to tertiary column indicates the simulation did not ever achieve the criteria described in the main text for identifying the onset of tertiary creep. However, all these simulations did show an increasing creep strain rate by the final successful load step

Stress level (MPa)	Time to opening, periodic (hrs)	Time to opening, block (hrs)	Time to tertiary, block (hrs)
60	25120	4060	40000
80	4060	2160	37000
100	3000	2990	>13300
120	1700	1750	>3930
140	594	1370	4430
160	269	356	>1330
180	70.4	100	>701
200	>24.6	62.4	>182

6 Complete Microstructural Model for Creep Deformation in Grade 91

This report documents the interactions of two major microstructural mechanisms governing the response of Grade 91 under creep conditions: growth and coalesce of cavities along grain boundaries (modeled by interface elements also including grain boundary sliding) and evolution of dislocations and other defects within grains (modeled by the crystal plasticity finite element method). Chapters 2 and 3 have reviewed their independent contributions to the creep response of Grade 91 within a microstructural cell model. This section presents the combination of the two physics-based models to capture the primary, secondary, and tertiary phases of Grade 91 creep response at 600 C. Emphasis is placed on the agreement of the model with experimental creep curves during all three phases at higher load levels, the prediction of creep life accounting for grain diffusional creep at lower load levels, and the resulting trends of grain boundary cavity growth that align with experimental observations.

In Section 6.1, the microstructural cell model and problem setup are briefly reviewed. A series of finite element simulations are performed in Section 6.1.1 using the calibrated grain and grain boundary model parameters at loads ranging between 100 MPa to 160 MPa. In Section 6.1.2, the cell average strain rate is decomposed into contributions from each mechanism at loads 100 and 140 MPa to determine the dominant mechanisms during primary, secondary, and tertiary creep. Differences in the trade-off of mechanisms occurring at lower loads 60 to 80 MPa are studied in Section 6.1.3, followed by comparison of minimum creep strain rates at lower stresses with data from Kloc et al. [27] as well as trends for cavity sizes and density reported by Wu and Sandstrom [17]. In Section 6.2, parametric studies are performed to determine that the hardening slip resistance in the crystal plasticity model is responsible for the long duration of primary creep as opposed to the grain boundary sliding mechanism. Conclusions about the modeling framework are drawn in Section 6.3.

6.1 Cell model creep response across a range of stresses

The primary benchmark case for evaluating the performance of the crystal plasticity model for creep response is the 100 grain cell model discussed in Chapters 2 and 3. The 3D cell model is a $(0.2 \text{ mm})^2$ cube-shaped domain containing 100 grains that is meshed with 10,402 quadratic tetrahedral finite elements, and 467 internal grain boundaries made from 3,921 interface elements. The crystal orientations in the 100 grains are sampled from a uniform texture. The boundary conditions on the cell consist of symmetry conditions on the faces $x = 0$, $y = 0$, and $z = 0$. The effectively incomplete periodic boundary conditions obtained through multi-point constraints (MPC) are applied on the other 3 faces of the cube. For the simulations herein, a uniform pressure is applied on the $z = 0.2 \text{ mm}$ face to represent the tensile creep loading. The stress is increased linearly during 10 steps at 0.01 hours per step to reach maximum load at 0.1 hours. This stress increase period is subsequently referred to as the “load ramp period”. The values of stress are set to 100, 110, 120, 140, and 160 MPa to correspond to the load levels investigated experi-

mentally by Kimura et al. [23]. The temperature is set to 600°C. The series of time steps following the load ramp period vary based on the approximate creep lifetime of the specimen and are listed in Table 3-10.

6.1.1 Calibration of material parameters against higher stress data

The multi-mechanism crystal plasticity model was calibrated in Section 3.4.1 to capture the primary creep response evident in the experimentally measured creep curves of Kimura et al. [23]. The material parameters for the crystal plasticity model are listed in Table 6-1, and the simulated creep curves for applied stress 100 to 160 MPa are provided in Figure 3-9. The strain rate for each load level overlays very closely onto the experimental data during the primary creep regime. The grain boundary parameters for growth and coalescence of cavities were then adjusted along the lines of Section 2.3.1.7 and Section 5.4 to produce a close fit for the tertiary regime, and Table 6-2 contains these parameters. In particular, the grain boundary viscosity η_b and penalty stiffness K_{lin}^{user} have been chosen for moderate degree of sliding and stable interface normal traction fields. The initial cavity size, number density, and growth parameters are within ranges of physical characterizations of Grade 91 from the literature summarized in Chapter 2.

Table 6-1. Material parameters for multi-mechanism (CP) model

Property	Value	Units
E	150,000	MPa
ν	0.285	dimensionless
τ_y	40.0	MPa
τ_v	12.0	dimensionless
n	12	dimensionless
θ_0	800.0	MPa
m	1	dimensionless
D_η	1.2×10^{-9}	$\text{MPa}^{-1} \cdot \text{s}^{-1}$

Table 6-2. Material parameters for traction-separation rate equations and units

Property	Value	Units
η_b	1.0×10^6	$\text{MPa} \cdot \text{hr} \cdot \text{mm}^{-1}$
K_{lin}^{user}	1.0×10^8	MPa/mm
a_0	5.0×10^{-5}	mm
b_0	0.06	mm
D	1.0×10^{-15}	$\text{MPa}^{-1} \cdot \text{hr}^{-1} \cdot \text{mm}^3$
ψ	$15\pi/36$ ($= 75^\circ$)	radians
Σ_0	200	MPa
F_N/N_I	2.0×10^4	dimensionless
$N_{\max}/N_I$	1.0×10^3	dimensionless
β	2	dimensionless

Figure 6-1 examines the evolution of creep strain rate of the cell model as a function of time for various load levels. For the load level 140 MPa, the simulated strain rate history appears almost identical to the experimental curve from Kimura et al. [23] during the entire test duration. At the lower load levels, the minimum strain rate is over-predicted by a factor of two or less, and the experimental curve for 160 MPa has a faster acceleration than the simulated curve. The time elapsed to minimum creep rate is more closely captured by the model. The stress dependence of the cavity nucleation rate, controlled by the parameters β and Σ_0 , help to improve the closeness of the fit, as discussed in Chapter 2.

Figure 6-2 presents the history of accumulated strain of the cell model for each load level. Note that the measurements of “strain” for the test specimens are typically measures of the change in length of a gauge section. Thus, the very low strain values during the first hour of test can include other effects such as slip in the grips and local stress redistribution within the specimen that are not accounted for in the cell model. After these trends settle out in 1 to 10 hours, the simulated strain evolution agrees very well with the experimental evolution. The maximum strain level before divergence of the numerical simulations are about 1-2 % strain, while the tests typically reach 20% strain accommodated by necking. Detailed investigations of the cell model solution fields in Section 2.2.1.4 and Section 6.2 reveal that significant cavity growth has taken place by the time 1% overall strain is reached, so that the model is capturing the onset and early stages of damage during tertiary creep. Overall, the microstructural model with combined grain and grain boundary deformation mechanisms fits the experimental creep curves quite well considering the typical level of scatter in such experiments.

6.1.2 Decomposition of strain rate into deformation mechanisms

The overall deformation of the microstructural cell model recorded in Figure 6-1 is a combination of several active mechanisms in the grains and grain boundaries, and each of these features are represented by many finite elements that are each in a separate kinematic and kinetic state. To more deeply probe the contributions to the total observed strain rate, domain-average values of strain rate are computed for the solid finite elements and interface finite elements, separated by

mechanism. All of the strain-like quantities are evaluated as tensors, and the axial component of strain rate $\dot{\epsilon}_{xx}$ is reported in the figures that follow.

The dislocation creep rate $\bar{d}^p$ from (3.57) and the diffusional creep rate d^d from (3.58) are provided directly by WARP3D for each solid element in the model as a state output at each time step. These values are integrated over the domain to compute the volume average. The total strain rate for grains is computed from the finite difference of the elemental strain field, and the elastic strain rate is found by subtracting the dislocation and diffusion tensors from the total rate tensor.

Details for the derivation of interfacial strain rates due to grain boundary opening are given in the literature in [12]. The resulting expression for strain, valid at small deformations, is:

$$\epsilon_{ij} = \frac{1}{2V} \sum_k^{g.b.e.} \left[\int_{S_i^k} \llbracket u_i \rrbracket n_j + \llbracket u_j \rrbracket n_i ds \right] \quad (6.1)$$

where the summation is over all grain boundary elements (g.b.e.), and V is the total volume of the cell. For each interface element, this tensor is decomposed into a component aligned with the unit normal vector of the element (representing opening) and a component lying in the plane of the element (representing sliding). These decomposed tensors, which have a spatial orientation, are then integrated over the domain and the uniaxial component is recorded. While these formulas are approximations, they provide adequate and useful insight into the dominant deformation mechanism at different times during the cell model creep response.

The decomposition of the cell average strain rate was investigated for specific load levels: 140, 100, 80, and 60 MPa. Figure 6-3 examines the decomposition at the 140 MPa load level, where the “Total” curve matches with the respective curve in Figure 6-1. Several distinct phases are evident at the higher applied load levels. During the load ramp period and shortly after, the elastic strain rate in the grains and the sliding along grain boundaries dominates the total cell deformation, up to about 1 hour. Then, the strain rate from sliding continues to decrease by several orders of magnitude over a long period of time, with the transition at 2 hours of grain dislocation creep labeled as “Gra. – plast” becoming the largest component of the total strain rate. Grain boundary sliding continues along a curve that is parallel to the grain strain rate, with a strain rate about one third of that in the grains. During this period, the strain rate due to grain boundary opening labeled “GBs – opening” continually decreases and is several magnitudes below the other components, indicating that only the penalty or elastic part of the grain boundary opening is occurring. At 100 hours, the opening rate begins to increase, most likely corresponding to the onset of cavity nucleation and growth at faster rates. This is the first component to show accelerating strain rate, and it occurs about 700 hours before the observed overall minimum strain rate of the cell model. The second component to accelerate is the grain boundary sliding, signifying that boundaries are likely relaxing from the additional opening displacement and allowing more sliding to take place. Lastly, the grain creep strain rate accelerates after 1000 hours is reached; this may be attributed to redistribution of stress between grains due to failed grain boundary facets with large cavity populations that no longer transmit much traction across the microstructure.

Note that because of the large applied load, the strain rate due to diffusional creep in the grains is $2 \times 10^{-7} \text{ hr}^{-1}$, which is the lowest mechanism contribution to the total cell strain rate.

Figure 6-4 presents the strain rate decomposition at the superimposed load of 100 MPa. Similar trends appear as for the 140 MPa case; the fraction of total deformation due to grain boundary sliding remains as one third of the grain strain rate during the later portion of primary creep. The transition from sliding to dislocation creep as the dominant mechanism occurs near 10 hours. The sequence of accelerating strain rates, with opening followed by sliding followed by dislocation creep, is again present. The explanation due to unlocking of boundary deformation followed by stress shifting to grains along alternative load paths is a logical explanation of the sequence of mechanisms apparent in the strain rates. Lastly, diffusional creep is a much larger fraction of the total rate at the 100 MPa load level, about one tenth of the total at the time of minimum creep strain rate.

6.1.3 Prediction of creep response at lower stresses

The creep response of Grade 91 at operating stress levels is of interest for design of reactors. The duration of tests at these lower stress levels is often prohibitive, and therefore modeling of material response is desired. The material parameters calibrated in Section 6.2.1 and given in Table 6-1 and Table 6-2 are thus employed for a series of creep deformation simulations of the cell model with applied stress below 100 MPa. The load levels of 80, 70, 60, 30, 10, and 1 MPa are chosen because limited experimental data for minimum strain rate during creep tests exist for each of these loads [27] [75] [76] [77] [78]. The sequence of time steps for the 60 to 80 MPa simulations are listed in Table 3-10.

Table 6-3: Time step size for sequence of steps for various load levels; step size in hours, uniform during steps between the numbers in first column; last row is total simulation duration in hours

First series step	80 MPa	70 MPa	60 MPa
1	0.01	0.01	0.01
11	0.11	0.11	0.11
101	0.242	0.242	0.242
201	0.5324	0.5324	0.5324
301	1.17128	1.17128	1.17128
401	2.576816	2.576816	2.576816
501	5.668995	5.668995	5.668995
601	12.47179	12.47179	12.47179
701	27.43794	27.43794	27.43794
801	60.36346	60.36346	60.36346
901	132.7996	132.7996	132.7996
1,001	292.1592	292.1592	292.1592
2,000	316,496	316,496	316,496

First, the decomposition of strain rate during the time history of the cell model is studied for the 80 MPa load level, and the result is given in Figure 6-5. Several distinguishing features emerge compared to the behavior of the 100 MPa case in Figure 6-4. First, the transition of dominant mechanism from sliding to grain creep is later for the 80 MPa case, at 30 hours. Also, the dislocation creep rate is comparable to the sliding strain rate during much of the primary creep regime;

both of the curves have a similar slope of strain rate versus time. Most importantly, the diffusional creep within the grains exceeds the strain rate for dislocation creep after 2,000 hours, similar to the time at which the opening strain rate reaches its minimum value at 1,000 hours. The larger contribution from diffusional creep manifests in the total strain rate of the cell model by extending the period of secondary creep, the duration of which the strain rate is nearly constant. Note that the diffusional creep curve is constant after 0.1 hours, the ending of the load ramp period. This behavior agrees with the fact that the volume average stress on the cell model is constant over time because the total load does not change and small deformations are considered. The linear relation between diffusional creep strain rate and deviatoric stress implies that if the volume average of the deviatoric stress is constant, then the volume average of the diffusional creep rate is also constant.

Figure 6-6 presents the decomposed strain rates for the 60 MPa load case. More differences appear compared to the 80 MPa response. The strain rate contribution from dislocation creep is now lower than grain boundary sliding throughout the simulation, and it only exceeds the diffusional creep rate during a short period between 1 and 100 hours. The duration of the simulation lasts until nearly 300,000 hours, when the Newton-Raphson algorithm diverges. As with all cases before, the opening strain rate accelerates first at 2,000 hours, followed by grain boundary sliding at 10,000 hours, and lastly by dislocation creep at 80,000 hours. The dislocation creep strain rate increases relatively rapidly near the end of life, faster than any of the other mechanisms, although the logarithmic scale disguises the fact that the ten-fold increase occurs during 200,000 hours. The dominance of the diffusional creep as the largest strain rate contribution leads to a long period of secondary creep with a minimum strain rate of $1 \times 10^{-7} \text{ hr}^{-1}$ between about 200 to 100,000 hours.

The creep response of the cell model is reported for several lower stress levels in Figure 6-7 for the creep strain rate and Figure 6-8 for the accumulated strain. Note that the equation solver diverges at a similar total strain level of 1% to 3% strain for all of the load levels. As mentioned above, the creep rate curves become “flatter” at the lower stress levels due to the increased contribution from diffusional creep in the grains, which is assumed to have a time and strain history independent diffusion coefficient. Therefore, grain boundary sliding is the most significant contributor to the transient nature of the total strain rate, and the boundaries appear to relax the majority of the strain rate by the end of 10 hours, when the creep strain rate has decreased by 4 orders of magnitude from the initial strain rate at 0.1 hours (which includes the contribution from grain elasticity due to the applied stress increase during the load ramp period).

Figure 6-9 compares the predicted minimum creep strain rate as computed by the cell model to two experimental datasets [23] [27]. As mentioned in Section 3.3.2, the variation of minimum strain rate reported by Kloc et al. [27] demonstrates a clear shift in dominant mechanism near the load level 100 MPa. This trend is also captured in the simulated response from the cell model. Although the predicted creep rates are about half of those of [27], the slopes of the curves are parallel. This result is very important, considering that this dataset was not the target set for the calibration at higher stress levels. In particular, the simulation results for lower applied stresses of 1, 10, and 30 MPa are also included in Figure 6-9. The simulation results are also in the neighborhood of the data from Kimura et al. [23], with faster rates in some cases and slower in others.

Due to the change in slope on the logarithmic plot, which occurs between the stresses of 60 and 100 MPa, the behavior of the cell model is classified into two regimes: “dislocation dominated” for response above 80 MPa and “diffusion dominated” for response below 80 MPa.

Figure 6-10 presents the time to minimum creep rate as a function of applied stress. The time values for the simulations of the cell model are slightly longer than those from the experimental dataset [23]. Also, the variation of the simulation results appear to have a nonlinear relation of time to minimum versus applied stress for loads below 80 MPa.

Another distinguishing feature of the microstructural model with grain and boundary deformation mechanisms is that it can suggest transitions of dominant grain boundary cavity growth behavior at different levels of applied stress. Thus, the statistics of the grain boundary state variables are examined in a series of figures across the range of applied stresses considered in this report: 60, 80, 100, and 140 MPa.

Figure 6-11 presents the evolution of normalized cavity diameter and number density averaged across all grain boundaries in the model. Since the initial cavity size is 50 nm from Table 6-2 and the relative increase in size is about 10 to 20, the final cavity size is about 1-2 microns, which is comparable to observations of cavities in failed specimens of Grade 91 reported in Section 2.3.1.1.

Closely examining the normalized curves in parts (a) and (b) provides another important trend produced by the microstructural model. For applied stresses above 80 MPa, the cavity nucleation rate $\dot{N}$ is higher than the cavity growth rate $\dot{a}$ with this dominance increasing as the applied stress increases. For applied stress below 80 MPa, the reverse trend occurs; nucleation is slow relative to growth. By overlaying the black curves for 80 MPa in Figure 6-11 (a) and (b), the rates of cavity growth and nucleation are comparable. This change at 80 MPa correlates with the knee in the minimum strain rate vs. applied stress curve in Figure 6-9 both for the experimental and simulated creep response. Thus, the model predicts at higher stresses that a greater number of small cavities have developed by the time the specimen fails compared to lower stresses with fewer, larger cavities. This trend of cavity sizes as a function of applied stress has been observed in creep tests for 12% Cr steel by Wu and Sandstrom [17]. In particular, this source reports observing cavities at failure with maximum diameter around 2.5 microns for 90 MPa loading and 1.2 micron for higher stresses of 130 and 160 MPa.

Figure 6-12 examines the evolution of the maximum value of cavity size and number of cavities across all grain boundary elements. The lower stress levels require a longer time to reach the maximum number of cavities. Recall that the ratio $N_{\max}/N_i = 1000$ in Table 6-2, which is reached only for the grain boundaries at 140 MPa in Figure 6-12 (b). Another observation for the lower stresses of 60, 80, and 100 MPa is that the time at which the maximum number of cavities is reached is similar to the time that opening strain rate begins to accelerate for these models, a trend that is most easily seen by comparing with Figure 6-14 (a).

Figure 6-13 presents the percentage of grain boundary elements with ratio of cavity size to spacing of $a/b > 0.5$. This ratio is an indicator of cavity coalescence within a given grain boundary element. The curves for 60 and 80 MPa appear to be somewhat steeper, meaning that the cavities grow in size a bit more quickly in a relative sense. Also, similar to the trends in Section 2.3.1.6, the steepest portion of the $(a/a_0)_{\max}$ curves in Figure 6-12 (a) begin at instances in time similar to

the start of the respective curve in Figure 6-13. Thus, coalescence or the value of porosity reaching 0.5 appears to trigger the accelerated rapid cavity growth time period.

A final intriguing result is found by comparing the increase in cavity size to the time to minimum grain boundary opening strain rate, as shown in Figure 6-14. The horizontal line across Figure 6-14 (b) corresponds to a 2.5 increase in cavity size, from 50 nm to 125 nm. The elapsed time for 140 MPa load level for this growth is about 100 hours, which is also the time for minimum opening rate shown in Figure 6-14 (a) by the purple line. Similarly, the time of 3,000 hours for minimum opening rate of 60 MPa is not far from the 4,000 hour duration to 2.5 increase of cavity size. Note that the time to minimum opening rate greatly precedes the minimum total strain rate shown by the curves in Figure 6-7, although the change in slope from linear decreasing toward beginning of deceleration can help to discern this component strain rate. Another key point in Figure 6-14 (a) is that a straight line on the logarithmic plot passes very closely through the minimum strain rate points for all 4 load level curves, which spans across the mechanism transition for the grain deformation from dislocation creep to diffusional creep.

6.2 Investigation of grain boundary sliding contribution to primary creep

During preliminary investigations of the combined crystal plasticity and grain boundary models within the 3D cell simulations, the decreasing strain rate (primary creep) of the cell was found to depend upon both the amount of grain boundary sliding and the evolution of slip resistance within the grains. Examples of these overlapping contributions are visible in Figure 6-4 for the 100 MPa load case. Initially, the overall cell strain rate is about $4 \times 10^{-3} \text{ hr}^{-1}$ at 0.5 hours, and it quickly drops to $1 \times 10^{-5} \text{ hr}^{-1}$ at 10 hours. This drop in strain rate is associated with the blue curve for grain boundary sliding. After this time, the dislocation creep from the crystal plasticity model in the grains is the largest strain rate, and it also continues to decrease from $5 \times 10^{-6} \text{ hr}^{-1}$ to $5 \times 10^{-7} \text{ hr}^{-1}$ at 10,000 hours due to the increasing slip resistance $\tilde{\tau} = \tau_y + \tau_w$. Therefore, in order to determine a unique set of calibrated material parameters that accounts for these overlapping mechanisms, a parametric study of grain boundary viscosity was performed to understand whether sliding alone could account for the long durations of primary creep exhibited by the creep curves of Kimura et al. [23].

This series of simulations for the cell model considered geometrically nonlinear kinematics with an applied total tensile force representing 120 MPa on the undeformed cell cross-section. Cavity growth on grain boundaries was suppressed so that steady state creep strain rates would be achieved by the cell model, hardening in the grains was suppressed by choosing the flow modulus $\theta_0 = 10^{-6} \text{ MPa}$ and saturation stress τ_y , and the diffusional creep coefficient was specified as $D_\eta = 0$. Therefore, the only transient effects exhibited by the cell model can be attributed to grain boundary sliding alone. The reference strain rate is set to $\dot{\gamma} = 9.55 \times 10^{-8} \text{ hr}^{-1}$ along with the power-law exponent $n = 12$. Two values of initial slip resistance are considered: $\tau_y = 40 \text{ MPa}$ and $\tau_y = 75 \text{ MPa}$. Three levels of viscosity are compared: $\eta_b = 10^3$, $\eta_b = 10^5$, and $\eta_b = 10^7 \text{ MPa} \cdot \text{hr} \cdot \text{mm}^{-1}$. These levels are similar to the estimated range of physically realistic values for viscosity in Chapter 2.

Figure 6-15 examines the evolution of creep strain rate for the cell model for each of the six combinations of the slip resistance and viscosity. The three curves for $\tau_y = 75$ MPa, indicated by “t=75” in the legend, have the lower strain rates overall as well as slightly longer periods of transient strain rates. For the cases with $\eta_b = 10^3$ MPa · hr · mm⁻¹, the relaxation of grain boundaries is almost instantaneous within a fraction of an hour. At higher viscosity $\eta_b = 10^7$ MPa · hr · mm⁻¹, the relaxation is delayed the longest over a period of about 70 hours. However, this duration is much less than the period of primary creep exhibited by the experimental data [23], for example 2000 hours at 120 MPa in Figure 6-1. Note that for each pair of curves with equal viscosity, such as $\eta_b = 10^7$ MPa · hr · mm⁻¹ denoted as “v=1e7”, the initial portions of the creep rate curves overlap, suggesting that the initial deformation is concentrated into the grain boundaries while the grains deform mostly at constant rate. Also, each of the simulations with the same slip resistance ultimately converge to the same steady state creep strain rate at later times; the extended period of strain rate decay could be due to the nonlinear kinematics and the non-zero value of saturation stress τ_v .

The shape of the primary creep portion of each curve is concave downward on the logarithmic scale, suggesting that the sliding rate drops more rapidly as a larger percentage of grain boundaries slide into a locked position at triple points. Only a finite amount of sliding can be accommodated in the microstructure due to geometric constraint without additional normal direction opening of grain boundaries. Also, since a single value of viscosity is assigned to all grain boundaries, their relaxation rate is similar throughout the cell. Preliminary studies of the cell model with a statistical distribution of viscosity parameter among grain boundaries [12] showed that the duration of primary creep could be extended by a factor of two or four.

However, the experimental creep curves for Grade 91 reported by Kimura et al. [23] clearly show a period of primary creep lasting one to several orders of magnitude time longer than 100 hours. In contrast, other simulations with higher levels of viscosity, such as $\eta_b = 10^9$ MPa · hr · mm⁻¹ in Figure 3-15, are found to contain almost no grain boundary sliding since the high viscosity keeps the grain boundaries locked past the time at which creep rate increases due to slow cavity growth or increase in stress due to reduction in cell cross-sectional area. Thus, the contribution of GB sliding to transient strain rate effects in the cell model has a limited duration of 100 hours when the viscosity is in an optimal range of $\eta_b = 10^6 - 10^7$ MPa · hr · mm⁻¹. For low viscosity, the grain boundaries relax too quickly and become constrained at triple points, leading to stress concentrations and issues discussed in Chapter 4. For high viscosity, sliding is prohibited and does not begin before other mechanisms of deformation initiate. Therefore, the long durations of nearly constant slope of creep strain rate reduction in the experimental data are accounted for by other mechanisms in the microstructural modeling framework, namely the evolution of slip resistance in the crystal plasticity model.

6.3 Conclusions

This section presents the combination of the two physics-based models to capture the primary, secondary, and tertiary phases of Grade 91 creep response at 600 C: growth and coalesce of cavities along grain boundaries (modeled by interface elements also including grain boundary sliding)

and evolution of dislocations and other defects within grains (modeled by the crystal plasticity finite element method). Simulations of the cell model are conducted at several applied loads, and the resulting cell strain rates are decomposed to understand the fraction associated with each mechanism in the modeling framework.

The response of the 3D cell during the early period of the loading history is characterized by sliding of grain boundaries to cause local grain motion, rotation, and elevated stresses near surfaces of certain geometrically preferred strains. At the same time and over a longer period, reduction in mobile dislocation density and other dislocation processes within grains lead to decreasing creep strain rates over time. Both of these phenomena contribute to the accumulated creep strain of the cell. After an extended period, the heightened stresses along grain boundaries drive the growth of cavities which induce an acceleration of the cell creep strain rate. Individual grain boundaries begin to experience failure with the geometrical linking up of sufficient grain boundaries to create a rupture surface over the cell roughly transverse to the applied loading. The elapsed time and total accumulated strain prior to strain rate acceleration are dependent on the applied stress as well as whether dislocation creep or diffusional creep is the dominant deformation mechanism within the grains.

The following points summarize the key findings from these series of simulations.

- The calibrated material models for the grain and grain boundary models are first employed in simulations for remote applied tractions of 100, 110, 120, 140, and 160 MPa at 600°C. For the load level 140 MPa, the simulated strain rate history appears almost identical to the experimental curve from Kimura et al. [23] during the entire test duration. At the lower load levels, the minimum strain rate is over-predicted by a factor of two or less, and the experimental curve for 160 MPa has a faster acceleration than the simulated curve. The time elapsed to minimum creep rate is more closely captured by the model for all load levels. The maximum strain level before divergence of the numerical simulations are about 1-2 % strain, while the tests typically reach 20% strain accommodated by necking. Detailed investigations of the cell model solution fields reveal that significant cavity growth has taken place by the time 1% overall strain is reached, so that the model is capturing the onset and early stages of damage during tertiary creep.
- The total cell average strain rate tensor was decomposed into component mechanisms from grains and grain boundaries by numerically integrating the strain tensors associated with solid and interface finite elements across the cell model. The decomposition of the cell average strain rate was investigated for specific load levels: 140, 100, 80, and 60 MPa. Several distinct phases are evident at the higher applied load levels. During the load ramp period and shortly after, the elastic strain rate in the grains and the sliding along grain boundaries dominates the total cell deformation, up to about 1 hour. Then, the strain rate from sliding continues to decrease by several orders of magnitude up to 2 to 5 hours when the grain dislocation creep becomes the largest component of the total strain rate.

At the 140 MPa load level, the opening rate begins to increase at 100 hours due to the onset of cavity nucleation and growth. The second component to accelerate is the grain boundary sliding, signifying that boundaries are likely relaxing from the additional opening displacement and allowing more sliding to take place. Lastly, the grain creep strain rate accelerates after 1000 hours is reached; this may be attributed to redistribution of stress between grains due to failed grain boundary facets with large cavity populations that no longer transmit much traction across the microstructure. The explanation due to unlocking of boundary deformation followed by stress shifting to grains along alternative load paths is a logical explanation of the sequence of mechanisms apparent in the strain rates.

- The decomposed strain rates at lower applied stresses exhibit distinguishing features compared to the 100 MPa case, the lowest load level reported in [23]. At 80 MPa applied load, the transition of dominant mechanism from sliding to grain creep occurs at 30 hours, while the transition is at 10 hours for the 100 MPa case. Also, the dislocation creep rate is comparable to the sliding strain rate during much of the primary creep regime; both of the curve have a similar slope of strain rate versus time. Most importantly, the diffusional creep within the grains exceeds the strain rate for dislocation creep after 2,000 hours, similar to the time at which the opening strain rate reaches its minimum value at 1,000 hours. The larger contribution from diffusional creep manifests in the total strain rate of the cell model by extending the period of secondary creep, the duration of which the strain rate is nearly constant. Under a 60 MPa applied load, the strain rate contribution from dislocation creep is lower than grain boundary sliding throughout the simulation, and it only exceeds the diffusional creep rate during a short period between 1 and 100 hours. The duration of the simulated creep response lasts until nearly 300,000 hours. As with all cases before, the opening strain rate accelerates first at 2,000 hours, followed by grain boundary sliding at 10,000 hours, and lastly by dislocation creep at 80,000 hours.
- The predicted minimum creep strain rate computed by the cell model is compared with two experimental datasets [23] [27]. The simulated response of the cell model captures the clear shift in dominant mechanism near the load level 100 MPa reported by Kloc et al. [27]. Although the predicted creep rates are about half of those of [27], the slopes of the curves are parallel. This result is very important, considering that this dataset was not the target set for the calibration at higher stress levels.
- Another distinguishing feature of the microstructural model with grain and boundary deformation mechanisms is that it can suggest transitions of dominant grain boundary cavity growth behavior at different levels of applied stress. Thus, the statistics of the grain boundary state variables are examined in a series of figures across the range of applied stresses considered in this report: 60, 80, 100, and 140 MPa. The average size of cavities along grain boundaries evolves from about 50 nm diameter to 1-2 micron diameter during the simulation, which is comparable to observations of cavities in failed specimens of

Grade 91 reported in Chapter 2. For applied stresses above 80 MPa, the cavity nucleation rate $\dot{N}$ is higher than the cavity growth rate $\dot{a}$ with this dominance increasing as the applied stress increases. For applied stress below 80 MPa, the reverse trend occurs; nucleation is slow relative to growth. This change at 80 MPa correlates with the knee in the minimum strain rate vs. applied stress curve both for the experimental and simulated creep response. Thus, the model predicts at higher stresses that a greater number of small cavities have developed by the time the specimen fails compared to lower stresses with fewer, larger cavities. This trend of cavity sizes as a function of applied stress has been observed in creep tests for 12% Cr steel by Wu and Sandstrom [17].

- Other corresponding trends have been observed between the decomposed cell strain rates and the grain boundary cavity states during the cell model creep simulations, for example by comparing the increase in cavity size to the time to minimum grain boundary opening strain rate. During the elapsed time of 100 hours for 140 MPa load level, the average cavity size grows from 50 nm to 125 nm, about a 2.5 increase in cavity size. The time at which the cell average strain rate begins to accelerate at 140 MPa also occurs at 100 hours. Similarly, the time of 3,000 hours for minimum opening rate of 60 MPa is not far from the 4,000 hour duration to 2.5 increase of cavity size; agreement is also observed for the 80 and 100 MPa load levels. Note that the time to minimum opening rate greatly precedes the minimum total strain rate, although the change in slope from linear decreasing toward beginning of deceleration can help to discern this component strain rate. Such agreements between macroscale quantities such as cell average strain and microscale quantities such as cavity distributions and sizes provide insights into the nature of deformation evolution in the microstructural cell model of Grade 91.
- Overall, the validated model suggests a clear creep mechanism shift from dislocation-dominated to diffusion-dominated at applied loads of about 100 MPa. This suggests methods for extrapolating creep properties from shorter-term experimental data to the long design lives planned for advanced reactor concepts may produce non-conservative results. This report considers 600° C. Physical arguments suggest that the mechanism shift will occur at higher stresses at lower temperatures and lower stresses at higher temperatures.

6.4 Chapter figures

Figure 6-1. Macroscopic cell strain rate (/h) versus model time (h) for cell model using calibrated material parameters including dislocation creep and diffusional creep within the grains and sliding and cavity nucleation along grain boundaries, compared to experimental data from Kimura et al.

Figure 6-3. Macroscopic cell strain rate decomposition into mechanisms within the grains and along grain boundaries at superimposed load level 140 MPa

Figure 6-4. Macroscopic cell strain rate decomposition into mechanisms within the grains and along grain boundaries at superimposed load level 100 MPa

Figure 6-5. Macroscopic cell strain rate decomposition into mechanisms within the grains and along grain boundaries at superimposed load level 80 MPa

Figure 6-7. Macroscopic cell strain rate (/h) versus model time (h), model predictions for creep response at reduced load levels below 100 MPa

Figure 6-8. Macroscopic accumulated strain (mm/mm) versus model time (h), model predictions for creep response at reduced load levels below 100 MPa

Figure 6-9. Variation of minimum creep strain rate with respect to applied stress from cell model compared to experimentally obtained rates for Grade 91 tests at 600 C from Kimura et al. and Kloc et al.

Figure 6-10. Variation of time elapsed to minimum creep strain rate with respect to applied stress from cell model compared to experimentally obtained rates for Grade 91 tests at 600 C from Kimura et al.

Figure 6-11. Effect of applied load level for constant material parameters on (a) average cavity size (across all grain boundary integration points), relative to initial cavity size and (b) average number of cavities (across all grain boundary integration points), relative to initial number of cavities

Figure 6-12. Effect of applied load level for constant material parameters on (a) maximum cavity size (among all grain boundary integration points), relative to initial cavity size and (b) maximum number of cavities (among all grain boundary integration points), relative to initial number of cavities

Figure 6-13. Effect of applied load level for constant material parameters on percentage of grain boundary elements with $a/b > 0.5$

Figure 6-14. Effect of applied load level for constant material parameters on (a) time to minimum grain boundary opening creep rate and (b) time to average cavity size $(a/a_0)_{avg} = 2.5$

Figure 6-15. Macroscopic cell strain rate (/h) versus model time (h) during primary creep for different grain boundary viscosity η_b and grain viscoplastic initial slip resistance τ_y

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7 The Effect of Triaxiality: Notch Strengthening and Weakening

7.1 Background

Notched bar creep tests can show either longer or shorter creep lives when compared to a straight bar specimen. The former is called notch strengthening and the latter notch weakening. Materials are often characterized as notch strengthening or weakening depending on their behavior under some standard set of test conditions [79]. However, experimental results show that the response of a material to a notch can depend on notch geometry [80] [81] and test environment [82]. The notch sensitivity of a material has a practical design impact: for notch strengthening materials a designer can ignore the effect of stress concentration when designing against creep rupture under constant primary load, but for notch weakening the effect of the stress concentration must be considered. Therefore, it is important to establish the notch sensitivity of Grade 91 at different temperatures, loads, and notch severities to determine if it will be notch weakening under any realistic design conditions.

Previous results for Grade 91 and similar steels generally indicate that they are notch strengthening [4] [83] [84] but can transition to notch weakening for severe notches [85] and possibly at lower temperatures and stress levels [5]. To our knowledge, no one has directly observed notch weakening for moderate notches in Grade 91 either at low temperature or at low stress levels, but previous works have speculated such a transition might exist. Low temperature and low stress tests are difficult experiments as they necessarily take a long time to complete and there is therefore limited experimental data on Grade 91, or other materials, in this regime. However, new advanced reactor designs target 60 year design lives meaning if a transition to notch weakening behavior exists in Grade 91 it may eventually manifest and result in non-conservative designs.

This chapter applies the crystal plasticity model for creep deformation and rupture developed in this report to describe notch strengthening and weakening behavior in Grade 91. The results indicate that while Grade 91 is generally notch strengthening it will transition to notch weakening behavior at low stresses and creep rates and for very severe notches. This is an important result as it could indicate a need to account for notches in primary stress design methods. This chapter develops a simplified microstructural model that explains the full simulation results. This model hypothesizes an equivalence between more severe notches and lower stresses/smaller creep rates, suggesting a possible surrogate experiment to probe notch sensitivity at lower stresses by testing severely notched specimens.

7.2 Model setup

This chapter starts with the periodic RVE developed in Chapter 5. Simulations results using that RVE are nearly identical to the block RVE considered in the rest of the report for high stress loading, above 100 MPa, and secondary and tertiary creep properties are consistent between the two models for lower stresses. Therefore, the results from the periodic RVE are consistent with the block RVE, which in turn has been validated against experimental data in Chapter 6.

However, the periodic RVE does not reach the tertiary creep stage before failing due to numerical instability. Therefore, Chapter 5 introduced the time to GB opening as a surrogate meas-

ure of rupture life. This measure will be used in this chapter to assess the effect of notches on creep life.

Notch effects on creep life are often thought of in terms of stress triaxiality. Introducing a notch increases the stress triaxiality – the ratio of the mean stress to the effective stress – in the notched region. This change in stress state in turn is thought to trigger differences in the creep mechanisms active in the material, leading to notch effects. To model increased triaxiality this chapter applies a macroscale stress state described by

$$\boldsymbol{\sigma} = \sigma \begin{pmatrix} 1 & 0 & 0 \\ 0 & \frac{F-1}{2+F} & 0 \\ 0 & 0 & \frac{F-1}{2+F} \end{pmatrix} \quad (7.1)$$

where σ is the applied loading stress, i.e. the actual stress applied in the experiment, and F is the triaxiality ratio. Note that with this definition and for $F > 1$ and $\sigma > 0$

$$F = \frac{3\sigma_m}{\sigma_e} \quad (7.2)$$

with σ_m the mean stress and σ_e the effective stress.

The transverse stresses are applied through the dummy degrees of freedom, as described in Chapter 5. They are increased proportionally to the applied load and then held constant for the duration of the creep simulation.

This chapter considers a series of simulations to test the effect of triaxiality on the model at three different loading stresses: 60, 140, and 200 MPa. At each stress level, four simulations are added to the previous simulation results with no transverse stresses, producing results for triaxiality ratios of 1.0, 1.5, 2.0, 2.5, and 3.0. Table 7-1 shows the transverse stresses for each case, calculated using Equation (7.1). Material properties are those of the final, full model for Grade 91, described earlier in this report.

7.3 The effect of triaxiality

Figure 1-1 shows the effect of triaxiality on creep for the full model. The figure shows the creep rate versus time curve for each combination of load and triaxiality. In general, triaxiality tends to decrease the primary and, for the low load cases that undergo it, secondary creep rates. The next set of figures show the effect of triaxiality on the different deformation mechanisms included in the material simulations. Figure 7-2 and Figure 7-3 show the loading direction and effective strain rates for the 60 MPa case at the five different levels of triaxiality, broken down by mechanism. Figure 7-4 and Figure 7-5 show similar plots for 140 MPa and Figure 7-6 and Figure 7-7 similar figures for 200 MPa. In general, triaxiality suppresses all the deformation rates except the linear viscous grain bulk term designed to represent bulk diffusional mechanisms. However,

it particularly suppresses grain bulk plasticity, reducing its importance relative to the linear viscous deformation mechanism.

Table 7-1 summarizes the effect of triaxiality on the time to GB opening for the three different load levels. At the highest load, 200 MPa, the model predicts notch strengthening behavior for all the simulated triaxialities. At the intermediate load, 140 MPa, the model predicts notch strengthening for low to intermediate triaxialities, transitioning to notch weakening for high triaxiality ratios. Finally, at the lowest load, 60 MPa, the model predicts notch weakening behavior.

Figure 7-8 shows the general trend for time to opening as a function of stress. Figure 7-9 graphically summarizes the results described in the previous paragraph by plotting the time to opening as a function of triaxiality at the three loading stresses. The behavior described by Figure 7-9b and by Figure 7-9c has been experimentally observed: both pure notch strengthening for relatively high stress creep experiments [7] and a transition between notch strengthening and notch weakening behavior as triaxiality increases for intermediate stress levels [9]. The behavior shown in Figure 7-9a – pure notch weakening for low loads/creep rates – has not been observed experimentally.

If the predicted transition to notch weakening behavior at low stresses exists in the actual material it will have an impact on long service life reactor designs. Current design methods for primary load creep rupture assume notch strengthening behavior, allowing the designer to ignore the effect of stress concentrations. These results indicate that Grade 91 may transition to notch weakening behavior for low creep rates and severe notches, necessitating a change in design practice.

The transition between notch strengthening and notch weakening behavior occurs approximately at the load level where the model transitions from a crystal plasticity dominated response to a diffusion/linear viscous dominated response – approximately at 100 MPa. As shown in Chapter 6 this transition has been observed experimentally. This mechanism shift suggests a simplified model that captures the trends observed here for the full simulations.

7.4 A simplified microstructural model

Consider a representative polycrystal under the stress state described by Equation (7.1). For $F = 1$ the polycrystal is under uniaxial tension and as F increases so does the triaxiality. Consider only dissipative deformation in the grain bulk. The simulations consider two mechanisms: the crystal plasticity model designed to represent dislocation motion and the linear viscous term designed to represent bulk diffusion. The average strain rate in the polycrystal is then

$$\langle \dot{\epsilon} \rangle = \langle \dot{\epsilon}_{diffusion} \rangle + \langle \dot{\epsilon}_{dislocation} \rangle \quad (7.3)$$

where $\langle \rangle$ indicate an average over orientation space. The diffusional term has no orientation dependence and can be represented as linear viscous deformation:

$$\langle \dot{\epsilon}_{diffusion} \rangle = k_1 \sigma \quad (7.4)$$

This is the exact form used in the simulations and a reasonable approximation for general diffusive mechanisms in the real material. The dislocation contribution might be approximated as power law slip on each slip system:

$$\langle \dot{\mathbf{e}}_{dislocation} \rangle = \left\langle \sum_{i=1}^{n_{slip}} k_2 \left[|\Sigma_i : \mathbf{M}_i|^n \text{sign}(\Sigma_i : \mathbf{M}_i) \right] \mathbf{M}_i \right\rangle \quad (7.5)$$

where the sum is over each slip system, Σ_i is the stress in grain i , $\mathbf{M}_i$ is the system Schmid tensor in sample coordinates, i.e.

$$\mathbf{M}_i = \mathbf{g}^T \text{sym}(\mathbf{b}_i \otimes \mathbf{n}_i) \mathbf{g} \quad (7.6)$$

with $\mathbf{b}_i$ the slip direction, $\mathbf{n}_i$ the slip plane normal, and $\mathbf{g}$ the orientation rotation, and $\left[\right]$ the Macaulay brackets.

To simplify the final model consider the Sachs approximation that the stress in each grain is the macroscale, applied stress:

$$\Sigma_i = \sigma \quad (7.7)$$

Classically, the Sachs hypothesis is a poor choice for crystals with a large number of independent slip systems as it will result in some systems with unrealistically high activation compared to others. However, for power law behavior in rigidly connected grains creep will tend to equalize the stresses in the different grains and so the Sachs approach may be reasonable for the long-term creep state of a polycrystal.

Now assume that the polycrystal will creep rupture when it reaches a critical amount of dissipated work:

$$W_f = \int_0^{t_{life}} \sigma : \langle \dot{\mathbf{e}} \rangle dt = \int_0^{t_{life}} \left\{ k_1 \sigma : \sigma + \left\langle \sum_{i=1}^{n_{slip}} k_2 \left[|\sigma : \mathbf{M}_i|^n \text{sign}(\sigma : \mathbf{M}_i) \right] \mathbf{M}_i \right\rangle : \sigma \right\} dt \quad (7.8)$$

This expression simplifies to

$$W_f = \int_0^{t_{life}} \left\{ k_1 \phi_1(F) \sigma^2 + k_2 \phi_2(F) \sigma^{n+1} \right\} dt \quad (7.9)$$

with

$$\phi_1(F) = \frac{3(2 + F^2)}{(2 + F)^2} \quad (7.10)$$

$$\phi_2(F) = \frac{\chi(F)}{\chi(0)} \quad (7.11)$$

and

$$\chi(F) = \left\langle \sum_{i=1}^{n_{slip}} \left[|\mathbf{D} : \mathbf{M}_i|^n \text{sign}(\mathbf{D} : \mathbf{M}_i) \right] \mathbf{D} : \mathbf{M}_i \right\rangle \quad (7.12)$$

with $\mathbf{D}$ the direction of stress

$$\mathbf{D} = \boldsymbol{\sigma} / \sigma = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \frac{F-1}{2+F} & 0 \\ 0 & 0 & \frac{F-1}{2+F} \end{pmatrix} \quad (7.13)$$

The function χ can be computed with an integral over orientation space. Figure 7-10 shows the factor ϕ_1 and Figure 7-11 shows ϕ_2 for a random texture and the BCC $[111] \times \{110\}$ slip systems used in the crystal plasticity model. ϕ_1 increases with triaxiality ratio. This makes physical sense as pressure, which increases with triaxiality, is a driving force for diffusion. ϕ_2 decreases with temperature, expressing the well-known principle that triaxiality suppresses plasticity. The values of ϕ_2 shown in the figure were computed via numerical integration over orientation space. However, $\phi_2 = 1 / F^5$ well-approximates the data.

Equation (7.9) can be cast as a model for rupture life:

$$t_{life} = \frac{W_f}{k_1 \phi_1(F) \sigma^2 + k_2 \phi_2(F) \sigma^{n+1}} \quad (7.14)$$

This tacitly assumes the material state remains fixed, which will not be true in the actual material. Nevertheless, the model adequately describes the interplay of dislocation and diffusion dominated processes causing notch strengthening and weakening in the simulation results.

Figure 7-12 sketches the effect of stress on the time-to-rupture predicted by the model for $F = 1$. A comparison to Figure 7-8 shows that the model captures the trends in the simulation data. Figure 7-13 then shows the predicted influence of triaxiality on rupture life for low, moderate, and high applied stress. For low applied stress the model predicts notch weakening, at moderate stresses the model predicts a transition from notch strengthening to notch weakening, and at high applied stress the model predicts notch strengthening. This agrees with the simulation results shown in Figure 7-9 and the functional form of the triaxiality dependence seems to agree with the simulation data.

The simplified model behavior can be described as a trade-off between dislocation dominated and diffusion dominated deformation. The key point is that diffusional deformation has a lower rate sensitivity exponent than dislocation dominated deformation and that triaxiality increases the rate pre-factor for diffusion but decreases it for dislocation motion. Because dislocation motion is more rate sensitive it will dominate at higher stresses and diffusional motion will dominate at lower stresses. The model predicts that triaxiality will decrease rupture life in the diffusion re-

gime and increase rupture life in the dislocation regime. Therefore at low stress, where the diffusional term governs, the material will be notch weakening. At high stress, where the dislocation term governs, the material will be notch strengthening. At intermediate stresses the two terms will result in a tradeoff between notch strengthening and notch weakening.

The model predicts that the transition between notch-strengthening and notch-weakening behavior is the same as the transition between dislocation-dominated and diffusion-dominated response. The full simulation results support such as a trade off as does the experimental literature (see Chapter 6). This provides a potential screening test to determine if a particular material in particular environmental and loading conditions will be notch strengthening or notch weakening: measure the effective rate sensitivity of creep deformation using short term, primary creep data and determine if the mechanism is diffusional ($n \approx 1$). If so, this simple model predicts the material will be notch weakening, particularly for severe notches.

As the above description shows, any model with the form of Equation (7.14) with an increasing ϕ_1 and decreasing ϕ_2 would qualitatively match the data. The advantage of the simple model here is that it provides an explicit way to calculate ϕ_1 and ϕ_2 so that the model includes the effect of texture and crystal system.

The model delimitates the notch strengthening and notch weakening regimes. Define the notch sensitivity of the material as the derivative

$$N = \frac{\partial t_{life}}{\partial F} \quad (7.15)$$

The material is notch strengthening if $N > 0$ and notch weakening if $N < 0$. Making the approximation that $\phi_2(F) \approx 1/x^5$ then

$$N = \frac{W}{\sigma} \frac{\frac{12k_1\sigma(F-1)}{(2+F)^3} + \frac{5k_2\sigma^n}{F^6}}{\left(\frac{3k_1\sigma(2+F^2)}{(2+F)^2} + \frac{k_2\sigma^n}{F^5} \right)^2} \quad (7.16)$$

which can be used to map the boundary between notch weakening and notch softening as a function of loading stress and triaxiality. This boundary is:

$$\frac{12k_1\sigma(F-1)}{(2+F)^3} + \frac{5k_2\sigma^n}{F^6} = 0 \quad (7.17)$$

or

$$\sigma = \left(\frac{5}{12} \right)^{\frac{1}{1-n}} \left\{ \frac{k_2(2+F)^3}{k_1(F-1)F^6} \right\}^{\frac{1}{1-n}} \quad (7.18)$$

As described above, one reason why notched tests are not commonly performed in low stress, potentially notch-weakening conditions is that the creep rates are low and the experiments take a long time to complete. The simple microstructural model developed here suggests an equivalence between low stresses and severe notches when testing for notch strengthening or weakening behavior. For example, when determining the constants k_1 and k_2 in Equation (7.18) experimentally a test procedure can either vary σ or F to generate the required data. The choice could be made based on the expected time required to rupture the specimen. Of course this assumes that only two mechanisms, dislocation-based and diffusion-based, influence the deformation of the material.

7.5 Summary

This chapter explores the effect of triaxiality on the response of the crystal plasticity model for creep and creep rupture in Grade 91 steel. The model predicts a transition between notch weakening and notch strengthening behavior in the material as either of the loading stress or triaxiality ratio vary. This implies that Grade 91 may transition to notch weakening behavior under low stresses/low creep rates/long creep lives, which would impact reactor structural design methods.

The chapter develops a simplified microstructural model for notch sensitivity that accounts for crystal system, texture, notch severity, and applied load effects. This simple model can be explained as the interplay of dislocation and diffusion dominated regimes of deformation. Future work will examine this model in relation to existing experimental data and previous theories of notch effects.

7.6 Chapter figures

Figure 7-2. Opening strain rates at 60 MPa showing the effect of triaxiality.

Figure 7-3. Effective strain rates at 60 MPa showing the effect of triaxiality.

Figure 7-4. Opening strain rates at 140 MPa showing the effect of triaxiality.

Figure 7-5. Effective strain rates at 140 MPa showing the effect of triaxiality.

Figure 7-6. Opening strain rates at 200 MPa showing the effect of triaxiality.

Figure 7-7. Effective strain rates at 200 MPa showing the effect of triaxiality.

Figure 7-10. Parameter ϕ_1 describing the effect of triaxiality on the linear viscous term designed to approximate the effect of diffusional deformation mechanisms.

Figure 7-11. Parameter ϕ_2 describing the effect of triaxiality on plasticity through the crystal system and material texture.

Table 7-1. Time to minimum GB opening rate for several stress levels comparing the periodic and block simulations. The table includes a column for time to the start of tertiary creep, which could only be reliably computed for the block models. A > symbol in the time to tertiary column indicates the simulation did not ever achieve the criteria described in the main text for identifying the onset of tertiary creep. However, all these simulations did show an increasing creep strain rate by the final successful load step.

Stress level (MPa)	Triaxiality ratio	Transverse stresses (MPa)	Time to opening (hrs)
60	1.0	0.0	25120
“	1.5	8.55	25120
“	2.0	15.0	23260
“	2.5	20.0	22775
“	3.0	24.0	22775
140	1.0	0.0	594
“	1.5	20.0	1520
“	2.0	35.0	2200
“	2.5	46.7	1900
“	3.0	56.0	655
200	1.0	0.0	>24.6
“	1.5	28.5	74.0
“	2.0	50.0	114
“	2.5	66.8	156
“	3.0	80.0	201

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8 Summary and Conclusions

8.1 Summary

The key results of this project to date are:

- A complete microstructural model for creep deformation in Grade 91 at 600° C. The model represents grain bulk deformation with a composite model including a slip-system-based crystal plasticity contribution representing dislocation-mediated creep and a linear viscous, isotropic term homogenizing the diffusional processes occurring along the sub-PAG defect network. The report validates this model against the available experimental data for Grade 91: complete creep curves at high stress and primary creep rates at lower stresses. This validated model incorporates developments and lessons learned in prior reporting periods into a tool that can predict low-stress, long-life creep properties of Grade 91.
- The model predicts a mechanism shift between diffusion and dislocation dominated creep occurring at 100 MPa at 600° C. This mechanism shift changes the shape of the predicted creep curves and manifests as a change in trend on plots of minimum creep rate and time to tertiary creep versus load. This mechanism shift may affect the accuracy of conventional methods of extrapolating high stress, short-term creep data to long-term properties, impacting the design of advanced reactors.
- Short term experiments generally show Grade 91 to be notch strengthening. However, the microstructural model predicts that is only generally true for high axial stress. For moderate axial stresses the model predicts a transition from notch strengthening to notch weakening as the severity of the notch increases. In the low stress, long life, diffusional regime the model predicts notch weakening behavior. If confirmed by experiments this would have a significant impact on long design life reactor designs as conventional design methods assume notch strengthening behavior.

Other results of this reporting period are:

- Improvements to the numerical implementation of the grain boundary model, increasing the numerical stability of the overall simulation framework and allowing the simulations to progress further into the tertiary creep regime.
- The composite crystal plasticity/linear viscous model for grain bulk behavior. This approach compares favorably to a dislocation density-based model implemented during the prior reporting period.
- A study showing that the block-sided RVE and boundary conditions used in these simulations have only a limited effect on the homogenized results when compared to true periodic cells and boundary conditions. Differences between the two approaches are only no-

ticeable in the primary creep regime of low stress simulations and can be attributed to artificial confinement of GB sliding on the block RVE faces.

- A software package for inserting cohesive elements on grain boundaries in true periodic RVEs.
- An exploration of numerical issues at triple points in simulations including GB sliding. Choosing an appropriate penalty stiffness can mitigate the near-singular tractions and oscillating stress fields developed by contact conditions at triple points.

8.2 Future work

Potential topics for future work and improvement of the simulation framework include:

- Extending the model to include the effect of temperature. This may be relatively straightforward – both the diffusional and dislocation/slip terms are thermally activated and the temperature scaling of such models is well known. Simplified models, like the type used in Chapter 7 to describe the effect of triaxiality, can also be used to reduce the required computational effort to simulate a wide range of temperature/stress combinations.
- Validation of the predicted transition between notch strengthening and weakening and the extension of the simple model to other materials. Other structural materials included in advanced reactor designs may show a similar switch to notch-weakening behavior at lower stresses and higher temperatures.
- A more accurate representation of diffusional effects. The current model homogenizes all diffusional deformation mechanisms into an isotropic, linear-viscous term. This is a good first approximation but a better model would explicitly model at least some of these mechanisms. Furthermore, even the treatment of diffusional void growth in the GB model is approximate as it is based on the periodic analysis of a single void cell. A multiphysics model could explicitly represent vacancy transport and couple it to the physical response of the grains and grain boundaries.

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